

# The Philosophy of Chemistry

The Philosophy of Chemistry:  
Practices, Methodologies, and Concepts

Edited by

Jean-Pierre Llored

**CAMBRIDGE  
SCHOLARS**

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P U B L I S H I N G

The Philosophy of Chemistry: Practices, Methodologies, and Concepts,  
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TO ROM HARRÉ, MICHEL BITBOL,  
MARINA BANCHETTI-ROBINO,  
AND MY PARENTS

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Nobel laureate in Chemistry	

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## PREFACE

ROALD HOFFMANN

From its beginnings, chemistry has posed a problem for philosophy. Why? Because this science, or the set of transformative protochemical crafts that comprised it before it became a science, did not fit well into philosophical categories, at least. Chemistry dealt with matter, and with its transformations. Quantification, better said measure, mattered – witness the papyrus recipes for indigo dyeing, the medieval prescriptions for making soap, or, still later, the signed protocol of Lavoisier's experiments decomposing and reconstituting water. But somehow change, the Heraclitean turn, rather than measure was (and is) the defining life thread of chemistry. Changes are often slow, as in the cycles of life. What impressed was dramatic change – the red crust formed on mercury heated in air, the way, still impressive today, that salt differs from sodium and chlorine.

There was certainly a place for matter and its transformations in an Aristotelian, experience-rooted world view – but less so when quantification took prime place. As Michael Weisberg has said, 'The problem for chemistry (and biology) in a post-Cartesian/Newtonian/Kantian philosophical world is that it looks a little too much like alchemy and not enough like Science.' Some of chemistry fit the quantifying mold. Or could be made to fit. But the defining bold changes never did fit, I think. And neither did the way chemists dealt with acquiring knowledge, especially when the microscopic perception of inner atomic and molecular structure became important. Lacking microscopes to reveal inner structure, in wonderful ways of knowing without seeing, moving ahead on meager clues, making molecule C from molecule B, that in turn from molecule A, all without really thinking through the ambiguities of the supposed knowledge of A or B – all that could be exasperating, or so I imagine, to those steeped in sound epistemological analysis. It was almost enough to put a philosopher in bed with a social constructionist of science.

We have come some way out of this initial quandary, and as these volumes, recent conferences, and much good thought and writing show, philosophy is in the midst of a real encounter with chemistry. The inherently synthetic nature of the chemical enterprise is being recognized,

with its special consequences, with links to ethics and aesthetics. As is the variety of ways in which chemical analysis proceeds. Even if people are still mostly talking past each other, applying only their own philosophical perspectives to the molecular science, there is a nice -- and fitting I think -- feeling of flux in the current philosophical discourse on chemistry.

Let me suggest some directions for the future philosophy of chemistry:

1. A recognition that the networks of communication of a field of knowledge shape understanding. And actually define the way the parts emerge from the whole. I have in mind the creative foment of the vast chemical literature, rivaled in the scriben (now word-processed) ways of knowing only by the biomedical literature. There is something organic here, the way chemical papers, read and cited, intertwine the way grass roots tangle and hold the soil. I have a feeling that the web of the literature is not only a communication device, but shapes individual actions, synthetic or analytical, in chemistry. That's also why it is so exciting (or frightening, for a chemist held back by conservatism rooted in age), to see changes in information technology affecting irreversibly the manner in which chemical information is communicated. Is there a philosophy of networks of knowing?

2. No question that reflection should be encouraged among a generally unreflective bunch of people in the trade. I am beating my own drum here, of course, but also pointing to chemists who have thought and written of their own world, people such as Pierre Laszlo and Jerry Berson. They are privy to the cognitive structures of the discipline, to Michael Polanyi's tacit knowledge. Polanyi himself was influenced in his philosophy, as Mary Jo Nye's recent book shows, by his own successes and failures in physical chemistry. The people I would urge the trade to encourage are chemists who *understand*, and if they also think about how and why they understand, this gives their work extraordinary value.

3. One can understand from the outside, too. Here is a welcome confluence of the history and philosophy of chemistry (or any science). For today's scientists have a very hard time getting into the mind-set of their predecessors. The cult of the new has them. Historians have cultivated the drive that empowers immersive patience, to learn the byways by which people thought a hundred or two hundred years ago. Larry Holmes's studies of Lavoisier's notebooks have led to important philosophical points about how chemical knowledge forms. In another context, the history of a phenomenon or concept in chemistry has to be taken into account in looking at any chemical work. If someone invokes "steric effects" or "aromaticity" as explanatory features, they are making connections with a historical tradition, one that may in turn have evolved;

aromaticity today has a different connotation from what it had a century ago.

4. Perhaps I am playing out my poetic predilection for seeing the world in a blade of grass, and just that drop of dew on that blade of grass, but I think that if we are to gain a philosophical understanding of chemistry today that we need more contemporary case studies. A detailed taking apart of a recent paper (and not yet another study of the Watson and Crick world-shaker) can be revealing in the extreme. One should read closely, with empathy for the authors' multifold struggle as they try to understand, to impress their colleagues, to convince.

By analyzing specific chemical papers with the full apparatus of philosophical thinking, seeing how the work functions as epistemology, narrative, and rhetoric, one gains insight into the complex world of the modern chemist. Reading closely several such papers leads to intimacy, a feeling that one knows how people think in the field. The philosophical background of the close reader of the individual work provides the analytical tools for adding value to this intellectual enterprise. For getting more out of those chemical papers than the people who wrote them, struggling for understanding, thought was in them.

If I were teaching a course in the philosophy of chemistry; I would ask each student to do a paper analyzing in depth a contemporary chemical article for the philosophical notions, explicit and implicit in each. And the study of recent papers might endow the metadiscourse of philosophy of science with one of the striking features of the subject, chemistry, itself. Which has added some 70 million compounds to what nature has provided us.

5. Both paradigmatic science and philosophy have trouble with the psychological, inherently subjective. My reflection on the remarkable network of chemists and chemistry is that the psychological intertwines with the logical, and that the fabric the two shapes is the way reliable knowledge and understanding forms. The facts are mute, and so, even within the confines of a tradition-bound mode of communication, a perforce subjective narrative of discovery and understanding must form. The scientific article, the conference (a 19<sup>th</sup> century creation, grown to epidemic proportions post-World-War II), create a constricting format in which people report work, claim priority and understanding, deny it. Citations are co-opted in creative, rhetorical ways. Psychological insight is needed to make sense of this playground of creation.

The psychological enters in another way, in shaping not only the aspirations of young chemists entering the field, but also the way they design their research, the questions they ask, and ultimately the proofs

they choose to provide for details in their chemistry. Virtue ethics, long neglected, has had a revival; “virtue science” may not even be defined. What I mean by the phrase is that young scientists (or older ones) model their work, sometimes subconsciously, on that of others they perceive as possessing innate quality, or gaining desired recognition. The outcome may laughable to bad – some scientists in China today imitating the hype level of their American protagonists. Some of it is much better -- R.B. Woodward or E.J. Corey serving as inspirations for two generations of synthetic organic chemists. My claim is that “virtue science” is pervasive. And that it influences the smallest level of scientific argument – for instance in looking for proof for a mechanism of a reaction in the detection of an intermediate more than in the kinetics of the process. With time, the small things, done originally in subconscious imitation, have a way of becoming the standard *modus operandi*.

Chemistry is cultural evolution at its best – human beings learning how to transform the natural, creating the new, and understanding the nature of these transformations on the microscopic and macroscopic levels. Some for good, some for... the less desired in us. It is important to think about how chemists gain or think their hard-won knowledge; how their tools, real and conceptual, affect their perception, and what they accomplish. I think philosophy, if it involves itself pragmatically in the realities of today’s chemistry, has much to add to our understanding of this beautiful way people have crafted of knowing and transforming the world.

## PREFACE

ROM HARRÉ

From its modern beginnings in the fifteenth and sixteenth centuries philosophy of science was comprised mainly of reflections on chemistry – the science of the transformation of substances from one kind to another – spontaneously or by manipulation. The works of Francis Bacon, Thomas Harriot, Robert Boyle, and John Locke are much concerned with the nature and possibilities of such transformations. The interest in changing one substance or a combination of substances into some new identity was the core of alchemy. Later, in the late seventeenth and eighteenth century's reflections on the nature of physics became more prominent – for example in the discussions on the nature of space and time that were the core of the discussions between Leibniz and Newton's 'front man' – Samuel Clarke. The laws of motion of the constituent atoms or corpuscles of matter as then conceived were those that had been developed by Galileo and Newton. Was chemistry already reduced to a branch of physics?

While this problem has been a fruitful meeting point between philosophy of chemistry and chemical theory and research there have been other important points of contact. How is it that molecules have properties some which are not shared with any of their component atoms – the problem of *emergence*? Chemistry is based on various *causal principles* and processes by which it establishes methods for analysing complex entities into their components. Causal interventions are developed by means of which the properties of material substances can be changed. Is the concept of causality in chemistry something unique to the science, or is it just a local version of more general causal concepts? From the beginning chemists have tried to set up *classification systems* to arrange the material stuffs of the world in coherent and useful ways. The final development of the classifying urge came in the periodic table of elements – and recent publications on this subject have shown just how complex are the philosophical problems that it raises. Does the role played by physics in proposing and testing hypotheses about the forces by which atoms are held together into molecular complexes show that chemistry as an autonomous

science with its own field of enquiry and its own methods of research could be and perhaps should be *reduced* to a branch of physics?

What can we learn as philosophers from the study of chemistry? Does the reasoning about parts and wholes that is central to chemical thought fit well with the standard rules of mereology, the logic of part-whole relations? For example, in mereology if A is a part of B and B is a part of C, then A is a part of C. Is this rule still valid when it comes to chemical wholes and their parts? Yet more recently another aspect of mereology has caught the attention of philosophers of science. It seems to be a basic rule of mereology that the products of an analytical procedure applied to some substance are to be treated as constituents of the substance from which they have been derived. There are many exceptions to this mereological principle and discussion of these exceptions has led to the importing of a new concept into philosophy chemistry – the affordance – what a substance displays on being acted on by a particular manipulation in a particular environment. According to the theory of affordances every type of manipulation produces its own type of affordances. Are electrons really constituents of molecules or must we conclude from the theory of molecular orbitals that it would be better to treat them as affordances?

The philosophical issues just outlined take their start from reflections on what chemists do and say and on studies of experimental manipulations and chemical theories. However it may be that chemistry can be used to throw light on issues that have arisen in general philosophy. A striking example is the question of whether there is any use in retaining a distinction between the real and the nominal essences of things and stuffs. What do kind terms like 'water' refer? Is it the everyday liquid which we use in ordinary life or does the growth of chemical knowledge oblige us to say that whatever may be the surface appearances of a liquid is only 'water' if it is 'H<sub>2</sub>O'? More precisely do the criteria of identity for water change when we know from chemical research that it is H<sub>2</sub>O? Of course, any chemist will tell you water is not H<sub>2</sub>O but a shifting collection of various molecules. Related to this debate is the question of the nature of properties on the substances we run across in everyday life, and bring into our laboratories for study. Are properties just the sensory appearances of things? Considering this question takes us into deep metaphysical and ontological waters – such as phenomenalism, logical positivism, and other general orientations in philosophy.

However, a new dimension of philosophy of chemistry has opened up with the realisation that the way our everyday lives are lived, whatever role in society we occupy and increasingly it seems where ever we are on the surface of the earth, the chemical environment is the key to many and

perhaps the most important aspects of human well being. We might call this interest 'social-chemistry'. How can chemists devise processes for the production of goods and services that are acceptable as contributions to the conditions of life? How can chemistry contribute to the immense task of repairing the damage to our environmental conditions by the exploitation of the chemistry of the past? Entering into ethics we might ask should chemists scrutinise any project they are recruited to carry through with attention to the effects its fulfilment might have on themselves and others? This issue was also raised again and again in the past and still is far from settled. Should our utopias be technical triumphs as prophets of the early 20<sup>th</sup> century, such as H. Wells thought, or is utopia to be brought about by curbing of the techno-urge to more and more sophisticated and elaborate devises for living?



# INTRODUCTION

JEAN-PIERRE LLORED

This volume originates from the international workshop in philosophy of chemistry at the CREA (Centre de Recherche en Epistémologie Appliquée) on Saturday September 11, 2010, in Paris. This meeting was supported by the Ecole Polytechnique, the CREA, and the Doctorate School of the Ecole Polytechnique. I thank all those institutions again for making this event possible.

First and foremost, I would like to introduce the road that leads from this workshop to the whole book so as to help readers understand what is actually at stake within this collective project.

It might be of interest to readers to understand how one chemist turned to philosopher of chemistry. I was first trained as a chemical engineer before becoming a French professor ‘agrégé’ in chemistry. I decided to resume my studies in philosophy from the outset in order to take distance from my current activities and to acquire a basic knowledge in philosophy. I am thus studying history and philosophy of science in parallel with my professional life. I obtained a master’s degree in history and philosophy of science under the direction of Bernadette Bensaude-Vincent, and I am now finishing my PhD work in philosophy under the supervision of Michel Bitbol at the Ecole Polytechnique and that of Isabelle Stengers at the Free University of Brussels.

Having the opportunity to meet most of the researchers in this field of studies, I envisaged inviting some chemists, historians, and philosophers of chemistry to take part in a round table of discussions of common interests in order: (1) to investigate some key chemical concepts, (2) to query how to study chemistry as a science, and (3) to encourage philosophers, chemists, and historians to enter into a constructive dialogue with one another. The Paris workshop partly crystallized those preliminary purposes.

Bernadette Bensaude-Vincent introduced this meeting by proposing a reflection upon the techno-scientific aspect of chemistry. In this respect, she explained what she calls the ‘impurity’ of chemistry. Eric Scerri then proposed an overall view of the philosophy of chemistry while pointing

out new potential roads to explore. Michel Bitbol and I developed a work based on the study of different chemical practices, past and present, in order to query how a relational form of philosophy can be developed and related to the chemists' works that we analyzed. Pierre Lazlo presented a study of the concept of 'transition state' from an historical standpoint. François Pépin, a French specialist of Denis Diderot, highlighted some aspects of Diderot's philosophy and demonstrated how to connect them with current philosophical debates about chemistry. Joseph Earley sharpened and deepened his previous work on chemical closures in which he proposed a philosophical understanding of how different chemical individuals can 'hold together' under certain conditions. Rom Harré introduced and further developed his concept of affordances within the framework of chemistry. In so doing, he also pointed out how the Wittengsteinian concept of 'hinge' could be of importance for the future of the philosophy of chemistry. Isabelle Stengers eventually summed up the whole day's work while providing interesting insights about chemistry, its history, its singularity from other sciences and especially from physics, and its new challenges from our society. An intense and helpful debate then took place between the different participants. Chemists (engineers, technicians, researchers, industrialists and scholars, and teachers), historians, philosophers, and many other researchers from various fields (biology, ecology, physics, material sciences, and sociology) were engaged in discussions about: (1) the autonomy of chemistry, (2) some metrological and ethical problems raised by current chemistry, (3) the role and the interest of cooperation between different types of expertise, and (4) the role of instruments in the history of chemistry. It was a very good day of positive discussions during which some ready-made answers were put aside in order to let people really express what they have in mind as regards their own activities. When we cease to identify ourselves to the roles we play within specific professional domains, the debate sometimes turns out to be genuine and done with simplicity!

My aim in setting up this meeting was also to ensure that philosophers who come from divergent philosophical backgrounds remain interconnected by means of fruitful debates, which would include chemists. Notwithstanding their differences we can go beyond them, because I believe that philosophers of chemistry who are working on analytical studies of aspects of chemistry can collaborate with those who are developing an historical epistemology of chemical practices. These perspectives offer many opportunities for a wider and deeper understanding of chemistry. Differences in approaches, methodologies, and concepts are a starting point for further enquiries. They are springs for creativeness.

Michel Bitbol then advised me to publish the proceedings of this workshop. I followed his advice, and I widened the scope of the volume by including many other historians, philosophers, sociologists, risk experts, metaphysicians, epistemologists, anthropologists, and chemists from all over the world. This enlarged team gave rise to the present volume. I thus assembled most of the different researchers I had previously met in different conferences with the hope of encouraging them to interact further with one another. In this respect, the networking of teams of research underpinned the project and remained always present in my mind.

Readers will not find any teleological scheme within this volume, nor will they find any research on consilience, the concept introduced by William Whewell. This book is even less an attempt to reduce the diversity of the various perspectives into a unique scheme. On the contrary, it tries to make those approaches *coexist* without any kind of assimilation. In doing so, we hope to express the heterogeneity of the different activities which are subsumed under the global label ‘chemistry’. This book tries to make further studies co-emerge in future research.

Chemistry is not solely a system of propositions, a social product, or a set of conventions or of practices, among other possible definitions. It is neither exhaustively social nor simply logical. It is both and more. There is no ‘logothetical’ primacy to use Gilbert Hottois’s turn of phrase (Hottois, 2004), nor is there primacy given to human interests and social constructions. Every experimental arrangement, every system of chemical equations, every complex of chemical problems, and every relation with the rest of the society demand to be investigated. We need to intensify an epistemology of *detail* that is to say a ‘distributed’ philosophy to use Gaston Bachelard’s turn of phrase in *The Philosophy of No* (Bachelard, 1940 [1968]). In this respect, the aims of the present volume are manifold, but the essentials are: (1) to strengthen international interactions to study chemical activities, and (2) to foster new approaches to encourage the debate about chemistry. We must pave the way for cooperation within which the existing approaches as well as the emerging ones will become related to one another in such a way that it will not be possible to privilege one aspect over another. They will stand in a binding reciprocal interaction. In brief, we seek to create a dynamic perspectivism whose *geometral* is chemistry. We need at the same time to understand this type of geometral and what we actually subsumed under the word ‘chemistry’. Is this word *the* unique reference of the activities that it encompassed or the result of a loose family resemblance to refer to the second Wittgenstein?

In his book, *Human Understanding*, Stephen Toulmin asserts that: “Men demonstrate their rationality, not by ordering their concepts and beliefs in tidy formal structures, but by their preparedness to respond to novel situations with open minds.” (Toulmin, 1972, pp. vii-viii) New ways of doing chemistry demand that heterogeneous teams of researchers work together in order to face new challenges concerning our lives from within the world that chemistry has done so much to reveal to us. In order to meet this demand, I have divided the book into three main parts and urged all the authors from the outset to fit their contributions into this global scheme.

The first part encourages current chemists to describe their workaday practices while insisting on methodological, metrological, philosophical, and epistemological questions related to their activities. In doing so, those chemists invite historians and philosophers to provide future developments. In a nutshell, this part is a call for forthcoming collaborations focused on *instruments* and *ways of doing chemistry*.

Some researchers were uneasy about taking part in this project, given the title reference to the philosophy of chemistry. But all of them agreed to contribute because they have been querying their own activity for a long time and because they have been looking for clarification about what they call some ‘dark aspects’ of their own work. The idea was thus to follow chemical current ramifications and take them seriously not only in their various manifestations but also by considering the *problems at stake* and the *contexts of ongoing projects*. This part thus asks questions such as: How do current chemists develop their knowledge? What can we learn from new chemical practices? What are the roots of their workaday modern creativity? What about their many strategies to describe the world as a network of interdependencies?

I believe that before commenting on the gap between the aims of chemistry and its social representations, and before announcing the rise of a new green and sustainable chemistry, we should make sure that we understand existing ways of doing chemistry. At the same time we should query the thresholds of meaning that exist in chemical discourses and their status in the economy of knowledge, their entanglement with the discursive systems of other sciences pure and applied, and their expectations of developments in the future. A return by philosophers to studies of laboratory practice is of interest. It paves the way for studies of local practices and unveils interactions between science, industry, society and even humanity in general. In turning to these studies many chemists, philosophers, and risk experts highlight and put into question some new faces of chemistry. In doing so, they consider both the operative and the

performative frameworks of chemistry that is to say the very possibility for chemistry to transform the world as well as its very ability to symbolize it.

Following this line of reasoning, Minh-Thu Dinh-Audouin, a French organic chemist working for the French journal 'L'Actualité chimique', first proposes an overall view of the current chemists' activities. This preliminary panorama encompasses soft chemistry, sustainable chemistry, and many other new chemical trends, and focuses its attention on the current process of reorientation and reshaping of chemistry. Sylvain Caillol, a specialist of sustainable chemistry and the director of the European chemical chair for a sustainable development CHEMSUD, studies how chemists reduce environmental impacts and above all how they contrive and develop new tools (concepts, devices, and so forth) in order to achieve this goal. In this respect, he scrutinizes what 'eco-design' means from within chemists' work while putting the methodology involved in the determination of a chemical 'life cycle' into question. He thus paves the way for an epistemological enquiry about the methods and the explanations used by chemists in such contexts of doing. Olivier Godard (expert in econometrics) then analyses how the precautionary principle can be connected with chemical risks. In doing so, he points out that there is no alternative but to pursue detailed investigations about the meanings of chemical risk assessments and the way by which they could be related to ethical questions. As a consequence, Godard studies chemistry envisaging its close dependence on norms, laws, political decisions, and social pressure.

Stéphane Bouchonet and Saïd Kinani, two experts in analytical chemistry, then ask the question of how new knowledge and know-how arise in analytical chemistry. They query how the couplings between analytical methods are achieved with the view to respecting norms and standards for the environment. In so doing, they raise the current problem of the meaning of their analysis in particular when chemists have to cope with the absence of a 'blank matrix'. It is the very process from which chemists give sense to their analytical results that, according to them, deserves to be looked at in somewhat more detail, and especially the way chemists define and prepare 'chemical references' which allow them to calibrate their methods and to quantify other chemicals. Their contribution to this volume was important because such methodological and metrological aspects of the chemists' work need to be further studied from an epistemological standpoint. Metrology and analytical procedures should enter into the epistemological domain of chemistry in so far as they are the 'hinges' around which all analytical reasoning turns. It is all the

more important that chemists never cease to set-up new couplings between methods in order to reach smaller quantities of compounds. The course of the environmental norms depends on such a current work.

The other contributors of this part bring to light that the coherence of chemistry as well as its 'margins' are constantly in question. Joachim Schummer, chemist and philosopher of chemistry, deepens the understanding of the role and the place of chemistry within the domain of nanotechnology. Jean-Baptiste Renard and Gwenaël Berthet, experts in instrumentation, query the interdependence of different specialties within the domain of the chemistry of the stratosphere. They provide the readers with metrological insights and reflections about interdisciplinary practical networks. Once again the instruments and the procedures are worth examining more closely in order to grasp what is at stake in current chemical activities. The same holds for the frontier between chemistry and biology. Gucki Riva Alessandra, Alain Hénaut, and Daniel Daugeron, three experts in biology, metrology, and instrumentation, investigate the current relations between chemistry and biology by focusing their work on the example of microarrays. They highlight how the trainings of the researchers and the different crossroads within particular projects of research were of paramount importance to understand the rise of such a new technique. They also explain how microarrays modified the practices of the scientists involved in such projects. The last team of researchers composed by Stéphane Sarrade (a chemist expert in sustainable process using supercritical carbon dioxide), Anne Aimable and Roberta Brayner (chemists respectively experts in ceramics and biomineralization), Mathieu Rozé (chemist expert in polymerization and material sciences), and I (chemical engineer and student in philosophy) investigate the role of interfaces in chemistry. In line with the French philosopher François Dagognet (1982), we focus our attention on the physicochemical interfaces as well as the interfaces between different specialties or those between scholars and industrialists from within a particular research program. As Joseph Rouse asserted: '[...] what results is not a systematic unification of the achievements of different scientific disciplines but a complex and partial overlap and interaction among the ways those disciplines develop over time.' (Rouse, 1996, p. 177) Interfaces push chemists to think about composition, arrangement, size, and structure at the same time. Interfaces also query Thomas Kuhn's concepts of paradigm and of scientific community. The last paper develops those aspects in order to express how the concept of interface is promising to envisage chemistry philosophically. Rom Harré's proposal of an open conclusion for the first part goes beyond its scope and paves the way for further

developments. He brings together instrumentation, affordances, and chemical mereology as key issues for further study in the future.

The second part of the book illustrates the multifarious ways to study chemistry and even proposes new approaches to do so. Each approach is interesting and incomplete but the emergent whole is richer than any of its components. Assembling without assimilating or reducing is not as unreachable as it is often alleged to be. It is nevertheless not a simple experience. Analytical works need socio-historical expertise as well as many other approaches in order to keep on exploring chemistry. Interfaces and flux between those approaches might turn out to be starting points for further philosophical investigations. This heterogeneity provides a wide set of perspectives not only about current chemical practices but also about the ways to explore them. Each approach is a *resource* to study chemistry and to reflect upon what *doing philosophy of science* can mean.

We need every expertise, from analytical philosophy to historical epistemology and from pragmatic approaches to neo-Kantian ones, to quote but a few. The different approaches offer opportunities for a deeper scrutiny of chemistry. The philosophy of chemistry more than ever needs to define international programs of research in order to make intellectual progress about the nature of science, human knowledge, and humanity. We need analytical philosophical approaches in the same way we need constructivist ones and other new perspectives. Those approaches are interdependent; their argumentation should co-evolve towards finer analysis. Their conjunction is possible and their articulation is necessary and always provisory. One of the positions that I would like to dwell on in some detail within this second part of the volume is precisely how every approach is of importance for the study of chemistry and how a wider understanding of chemistry *emerges* from their complementarity. Networking is a good way to make a group creativity emerge. Connecting researchers enables us to transform current approaches and to arouse thought gradually.

The second part is divided into six types of perspectives, which are as many ways of studying chemistry. This type of classification is always arbitrary and closer attention will easily reveal that those styles of work are not independent from one to another. Moreover, I do not claim any form of exhaustiveness. This ‘classification’ is merely a tool for framing my presentation while leaving open any connection between the approaches involved and possible forthcoming ones.

This second part first focuses on historical studies of chemical activities. Historicizing epistemology is still a challenge and the roads to achieve this historicization are multifarious and winding as Hans-Jörg Rheinberger has shown (Rheinberger, 2010). What remains nevertheless



important for this volume is to point out how historical surveys can provide philosophers with crucial elements in order to develop their own perspectives. At the same time, it is worth noticing the subtlety of the differences between those historical approaches. There is no unique way of doing history of science. Much depends on the topic being studied, the socio-political and cultural contexts, and the historians themselves. The following studies thus express various types of historical research that are useful for widening our understanding of chemistry. Eric Scerri (chemist and philosopher of chemistry) develops the topic of the lecture he delivered during the Paris workshop. Ana Simões and Kostas Gavroglu (historians of quantum chemistry and epistemologists) show how history enables chemists and philosophers to understand the chemical bond better. Marina Banchetti-Robino (historian and philosopher) draws her attention to the relevance of Boyle's chemical philosophy for contemporary philosophy of chemistry regarding questions related to reduction of chemistry to physics, emergence, and so forth. François Pépin develops the idea he proposed during the Paris workshop about Diderot's philosophy while stressing its interest for contemporary philosophy. Voillequin Baptiste (chemist, historian and philosopher of chemistry) queries historical methodology by evoking the case of catalysis in France. He refers to Latour and ethno-methodology. Dominique Pécaud (sociologist of science) uses history in order to develop 'a political form of epistemology' according to his own turn of phrase. To do so, he refers to Swift, Comte, Berthelot, and others, so as to study the relationships between agricultural chemistry and agriculture. The transformation of the world by chemistry remains at the very heart of Pecaud's work.

The second type of perspectives envisages chemistry as a 'techno-science'. This concept is used by Latour and many others to describe current scientific innovations and doings. It often raises controversies and passionate philosophical debates that invoke issues of ideology. Is a chemistry a techno-science and in which sense? What is the interest, if any, of such a concept regarding current chemical activities? How does this concept renew the understanding of science? Those questions and many others are open. In order to clarify the situation, Gilbert Hottois (philosopher), who first conceptualized and proposed the concept of techno-science, was asked to recall his initial understanding of this concept and to explain how he connects it with chemistry. Bernadette Bensaude-Vincent and Ursula Klein (historians and philosophers of chemistry) then develop their own different approaches. Bensaude-Vincent explains to what extent chemistry can be envisaged as a techno-science. Klein focuses her work on the relationship between materiality and



abstraction in modern chemistry. Once again, the diversity of approaches is at the very heart of this part in order to figure out what is at stake in this debate and to explain why chemistry has an important part to play in it.

The third type of perspectives envisages chemistry as a field of practices as well as a field of knowledge. This part can be partly related to what philosophers call the ‘practical turn’. Philosophers consider what chemists are doing (symbolization, conceptualization, creation of instruments, devices, synthesis of new chemical bodies, and so forth) in their everyday activities. Rein Vihalemm (philosopher of chemistry) asks the question: What is a Scientific Concept? He develops some considerations concerning chemistry in a practical realist philosophy of science in order to answer his question. He introduces a new form of practical realism. In line with the lecture that we gave during the Paris workshop, Michel Bitbol (philosopher of quantum mechanics) and I scrutinize different chemical practices in order to identify and to create a relational philosophy that fits them. Following Denis Diderot, the later Wittgenstein, and Roald Hoffmann, we aim to return to the laboratory as the centre of research and to create a philosophical approach from within chemistry. Our work is simply applying concepts that were developed in other domains on chemistry but takes chemistry as a starting point for a particular philosophy, if any. Pierre Laszlo (chemist and historian of chemistry) enters into more technical details about chemical analysis and describes the process of dematerialization related to them. Manuel Bächtold (physicist and philosopher of science) who cleverly develops a pragmatic approach of quantum physics proposes a pragmatic study of the atomic model in chemistry. Andrew Pickering (one of the ‘Pilgrim Fathers’ of the practical turn) then proposes an innovative paper entitled ‘The Tao of chemistry’ in which he emphasizes the process and the ongoing transformation of chemical practices as well as that of chemicals themselves. Flow and change are the cornerstones of his approach. Hasok Chang (philosopher of science) envisages the philosophy of chemistry as a complementary science. He explains how the history and the epistemology of chemistry enable philosophers and chemists to reopen their understanding of previous chemical failures in order to explore new chemical possibilities of action.

In the fourth types of perspectives, three prominent philosophers of sciences were invited to develop a transcendental approach for chemistry. Olimpia Lombardi and Mariana Córdoba propose a Kantian approach for the philosophy of chemistry and Sami Pihlström explains how it is possible to connect a pragmatically naturalized transcendental philosophy of science with the philosophy of chemistry. The conditions of possibility

of the chemical practices are stressed from within the context they are embedded in.

The fifth group of perspectives is related to analytical perspectives and metaphysics. Robin Findlay Hendry (philosopher of chemistry) develops three metaphysical issues in the philosophy of chemistry, that is to say issues about substances, structure, and their relation to reduction of chemistry to physics. Paul Needham (philosopher of chemistry) focuses his work on mereological structures in chemical substances and their transformations. In doing so, he proposes an analytic perspective on the historical development of these concepts. Once again, Paul Needham scrutinizes the parts/whole reasoning in chemistry with an astonishing sense of detail. Anna Ciaunica-Garrouy (philosopher of science), who has not previously worked on chemistry, was asked to adapt and to develop her promising work regarding the relations between the levels of organization by including chemical individuals into the topics of her reflections.

Joseph Earley was asked to propose an open conclusion for this whole second part. Stepping back, he has developed an astute reflection upon how those perspectives hold together.

In the last part of the volume, philosophers propose new concepts or reshape older ones in order to think about chemistry. In line with the lectures they gave during the Paris workshop: (1) Rom Harré develops the concepts of affordances and hinges in order to focus his work on the *interaction* between chemists and the world and to highlight how chemical knowledge and know-how revolve around ‘hinges’ in the Wittgensteinian meaning of this word. Those concepts are of paramount importance for thinking about our actions upon the world and the kind of knowledge scientists can reach as regards the world; and (2) Joseph Earley develops his three concepts of chemical closures and queries their epistemological significance. He proposes a way of developing a processual philosophy of chemical transformations within a second paper. José Chamizo (chemist) then proposes to reevaluate the concept of chemical experiment. Once again, doings and laboratories are the starting points for a new conceptualization. Isabelle Rico-Lattes (chemist) and Laura Maxim (expert in ecology and in communication sciences) explore chemical practices in order to develop the concept of ‘sustainable’ chemistry. They shape and deepen their concept from within their work developed on the terrain of environmental regulations (REACH). Alexandru Manafu (philosopher of science) then proposes a concept of emergence for chemistry. Michel Bitbol develops a new concept of downward causation without referring to any ‘foundations’. This paper is crucial in so far as it

provides philosophers of chemistry with new arguments to think about a whole, its parts, and the surroundings all at the same time. In this respect, Michel Bitbol's book *'De l'intérieur du monde'* might become a springboard for the philosophy of chemistry in general because of its understanding of the relations/*relata* interdependency (Bitbol, 2010). William Goodwin (philosopher of science) draws attention to the concept of structure and connects it with the question of reduction between disciplines. He exemplifies his statement by considering the relationship between organic chemistry and quantum chemistry. Last but not the least, Alfred Nordmann (philosopher of science and technology) develops the concept of 'metachemistry' by considering the specificity of technoscience and Bachelard's phenomenotechnique. He thus tailors a novel concept different from that of 'metaphysics'.

Let us consider this whole collective work as a simple *tool* tailored to encourage deeper and wider forthcoming works and to stimulate stronger cooperation. I hope that it will help this community of researchers to share their interests for chemistry with philosophers and researchers coming from other realms. I hope it will spark the interest of students in this domain of philosophy. In editing this volume I have aimed at respecting the diversity of the different approaches, as exemplified in the many books previously published in this field. More than ever we need to be open-minded in order to face the new challenges that chemistry imposes. Philosophy is derived from the Latin 'philo-*sophia*'. *Sophia* is always related to open-mindedness. In this respect, philosophy is a 'love affair', but a love of another kind that needs to be continuously transformed and adapted to the changing human contexts. To my mind, chemistry can provide philosophers and researchers in general with other tools in order to think about humanity, science, and our life in this world. It is precisely the theme of the global conclusion of this volume.

I would like to conclude this introduction by expressing my special thanks to the experts who gave me invaluable advice in order to improve and deepen this volume. I thus thank in alphabetic order: Anne Aimable, Marina Banchetti-Robino, Michel Bitbol, Anna Ciaunica-Garrouty, François Dagognet, Joseph Earley, Alessandra Gucki Riva, Rom Harré, Alain Hénaut, Roald Hoffmann, Pierre Lazlo, Muriel Le Roux, Olimpia Lombardi, Alexandru Manafu, François Pépin, Jean-Baptiste Renard, Eric Scerri, and Rein Vihalemm. I also thank the CREA, the Ecole Polytechnique, and its Doctoral School. I particularly want to thank Michel Bitbol for his trust, his advice, and his stimulating 'philo-*sophia*'. I would like to express my gratitude to Rom Harré for his generous and helpful presence. His deep philosophy gave me the energy to achieve this project. I thank

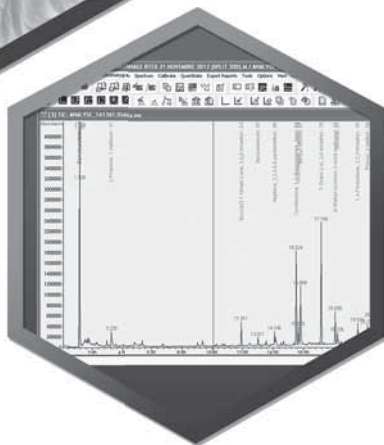
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# Exploring Chemical Practices *Part I*



# THE NEW CHALLENGES OF CURRENT CHEMICAL PRACTICES

MINH-THU DINH-AUDOUIN

At the dawn of a new millennium, the world is going through a major turning point. We realize that in thirty years the world population will reach nine billion; fossil resources are dramatically decreasing, agricultural areas as well as drinking water are lacking, and at the same time the planet is going through major transformations such as climate change. Meanwhile, poverty has not declined and inequalities in access to food, health care, housing and wealth remain a major global issue despite the huge scientific advances since the beginning of the industrial era, particularly in health, medicine and technology. Our human societies and environment will inevitably be confronted with abrupt changes within the next fifty years, and we will have to act rapidly in order to adapt to the upcoming world.

Probably more than ever, citizens have high expectations of the scientific community to find effective and sustainable solutions. As major actors in the industrial revolution, chemists play a leading role in that community and they are now facing new scientific and technological challenges, with unprecedented economic, political, social and moral pressure. Society is paying attention to that science of multiple facets, expecting a lot of chemistry, while still raising many questions.

Thus chemistry is arriving at an important and delicate turning point in its own history: the twentieth century scientific and technical advances and new societal needs will guide chemists in their research and lead them to change their practices and behaviors in a new global context. How do chemists work today and what is the impact on society?

## **1. Facing Environmental Issues**

The future of the planet is more than ever feeding debates in society. Industrial and scientific institutions, politics, non-governmental organizations and many citizens are mobilizing to find solutions to environmental issues. As a science focused on transformation of matter, chemistry is essential to understanding global scale phenomena (such as evolution of ecosystems,

interactions between air, soil and water, life cycles of matter, etc.), as well as to limit and prevent pollution or find sustainable resources and energies.

## **1.1. Searching for New Resources**

### **1.1.1. Biomass as an Alternative to Oil?**

Modern civilizations in the twentieth century have been developed by oil. That fossil resource is, however, about to run out and soon will no longer be sufficient to fulfill the increasing needs for heating, vehicle fuel and everyday life products. Nevertheless, nature is full of many other carbon sources that have been used for millennia: trees, grains, plants and algae, called biomass, are abundant renewable resources of organic molecules. These are large-sized, multiple and complex biomolecules such as cellulose, lignin, starch, vegetable oils or proteins that researchers have to extract from nature, characterize, split, transform and convert into biofuel or chemical intermediates which will be precursors of materials, food or medicines, whether new or already existing.

A new vast research field called “plant-based chemistry” (see *Formule verte*, le magazine des matières premières et des ingrédients renouvelables, 2010, 3; Dinh-Audouin 2011 and [www.chimieduvegetal.com](http://www.chimieduvegetal.com)) is opening for chemists today, eventually in continuity with oil chemistry, but moving towards processes increasingly respectful of human beings and environment (see paragraph 1.2.2): lots of work is being carried out to achieve processes with less emission of pollutants and greenhouse gas and to manufacture biodegradable products. Chemists are now facing the challenge to adapt bio-sourced products to future use: they have to define life cycles, biodegradability needs (speed, location, mode of degradation...), carbon footprint, etc. To succeed, collaboration with other disciplines is required: physics, biology, ecology, informatics (computing software...), etc. In the meantime, “white biotechnology” processes develop, often appreciated for low energy consumption, low pollutant emissions and remarkable efficiencies to transform biomolecules.

Biologists play an essential role by studying enzymes and microorganisms’ activity before implementing them in reactor plants; they have to collaborate with chemical engineers to solve many difficulties they meet to scale-up such reactions. Such collaboration is growing through the development of “biorefineries” (more than thirty in Europe in 2012), which are mostly small and medium enterprises (SMEs). Researchers from all over the world have taken up the ambitious challenge to develop that

new industrial branch: in Europe, the EuroBioRef project<sup>1</sup> (“European multilevel integrated Biorefinery Design for Sustainable Biomass Processing”) launched in March 2010. In France, many researchers work in the Axelera technopole with government agencies and industries to develop research in plant-based chemistry.

Could biomass become a sustainable solution for our resource limitations? One advantage is that the agricultural area required to produce chemical intermediates is rather small, with low competition with the food industry (unlike first generation bioethanol). Moreover, encouraging promises are coming from the advent of fast-growing trees to produce second generation biofuel from cellulose, or even third generation biofuel from algae. Today, bio-sourced products are commercially available, such as polylactic acid plastics produced by fermentation of corn starch on a one hundred thousand ton scale per year worldwide. That new generation of plastics is used in packaging with the advantage that they can be then composted.

So could biomass gradually replace oil? There are still lots of difficulties: it is both a scientific and industrial challenge, but also economic, social and political. For the first time, in a collective awareness of that new global challenge, a lot of actors from the worldwide society (academics, industrialists, teachers, politicians, economists, as well as marketing managers and environmental non-governmental organizations) are brainstorming concrete ways to develop plant-based chemistry, to identify new markets and to introduce associated values to the society.<sup>2</sup>

### **1.1.2. Oceans as an El Dorado of Mineral Resources?**

Most rich and available mineral sources have been exploited on the continents. But humankind did not wait for the urgent need for raw materials to start to explore the two-thirds of the planet still poorly known: oceans! For several decades, scientific explorers have been exploring the ocean depths beyond 2 000 meters, discovering mineral deposits containing an impressive variety of metals: iron, manganese, copper, zinc,

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<sup>1</sup> EuroBioRef project has been launched for a period of four years. It is coordinated by the Centre National de la Recherche Scientifique (CNRS) in France and involves 28 partners from fourteen countries, bringing together a wide variety of actors: chemical and biochemical (large companies and SMEs), universities, European organizations. See: <http://eurobioref.org>

<sup>2</sup> See: “Plant-base chemistry for 2020!” European symposium, September 5-6th, 2011, Maison de la Chimie (Paris). Organized by ACDV, Ademe, ERRMA, FNR, NNFCC, IAR, UIC. In: <http://www.chimieduvegetal.com>



gold, silver, cobalt, lead, barium, platinum, and titanium. These minerals, called polymetallic nodules, cobalt-rich crusts and hydrothermal sulfides, are formed in water with geological processes still poorly known.

More than scientific curiosities, these marine metallic sources now attract attention: scientists, industrialists and politicians might find a solution to raw materials' scarcity. Indeed, dense polymetallic nodules fields have been identified in the Clarion-Clipperton zone in the North Pacific, containing metals in equivalent or richer amounts than those of onshore fields. For example, nickel has concentrations at least equal to those of continental laterites<sup>3</sup>. Being aware of the potential economic importance of nodules and associated risks, geopolitical and environmental as much, President Johnson claimed in 1966 that the deep sea should be a "common heritage of humankind". The resolution was set in 1970 by the United Nations. In addition, cobalt-rich crusts contain more cobalt than continental exploited minerals. These resources are mainly used to produce special steels for new technologies, especially alloys for aviation and batteries, with an increasing demand. Furthermore, hydrothermal sulfides are estimated at millions of tons (see EDP Sciences 2009). The ocean floor is definitively full of treasures!

Is it possible to exploit them? Economic viability must be evaluated, and potential environmental impacts as well, because entire ecosystems with their biodiversity may be disrupted. Those aspects are closely monitored and regulated by the International Seabed Authority (ISA), which controls the exploitation of mineral resources in international areas. Researchers, such as geochemists and geophysicists of the 'Institut français de recherche pour l'exploration de la mer' (Ifremer) in France, in collaboration with other specialists of the sea, are conducting oceanographic surveys to gather field data (mapping, sampling, volume estimations) in order to understand the geological, chemical and biological processes that control the formation, size and diversity of minerals, and to study the possibilities for exploitation.

## 1.2. Environmental Protection

Modern societies benefit from major technological advances made possible through a better understanding of molecules, materials, their structures and properties. Nonetheless industrial developments raise the problem of large-scale waste and transport of huge quantities of products that have to be controlled; otherwise they may cause environmental and

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<sup>3</sup> Laterite is a rock rich in iron or aluminum hydroxides covering large areas of continents, which is formed by weathering of rocks in tropical climates.

human damages that could be irreversible. Tragic accidents regularly occurring generate a collective awareness of the need to develop a safer and cleaner industry. Scientists, particularly chemists, are at the forefront of developing techniques for treating polluted environments (water, air, soil), or better yet, providing upstream industrial tools and methods to help reduce all risk of pollution. Nowadays, when researchers develop chemical reactions, they are compelled to think of potential industrial applications with environmental implications. At the same time, industries face more and more responsibilities in Europe under the REACH regulation (Registration, Evaluation and Authorization of CHemicals) implemented since June 2007. They must evaluate and manage the risks of the substances they produce, both for human health and environment. That leads researchers to progress in the control of these risks and to provide safer processes and molecules of substitution. With the growth of knowledge and techniques in analytical chemistry, chemists have established efficient tools to detect molecules, to follow them in the environment, even in animals' bodies such as fishes (or even in the human body in order to study their toxic effects, as mentioned in section 2.2). Industry is becoming better equipped to control its effects on the environment. There is still a long way for REACH, as companies, particularly SMEs, to go so that they may meet technical, economic (employment of REACH managers, restructuring, costs, competitiveness) and legal issues. Furthermore, a possible extension to the global level might be hoped for.

### **1.2.1. Chemistry against Pollution**

In developed countries, drinking water is usually obtained thanks to treatment plants using physicochemical methods such as ultrafiltration (water is clarified and disinfected by retention of particles, algae and microorganisms by a passage through a microporous membrane under pressure), filtration through activated carbon (for example to get rid of some pesticides), disinfection with ozone or chlorine, or demineralization on ion exchange resins. Due to worldwide population growth and agricultural needs, water becomes scarce, especially in developing countries where it is often unfit for human consumption. The Global Program for the assessment of water resources, which was established in 2000 by the United Nations, has set a target of halving in 2015 the proportion of people having no access to safe drinking water. To meet this ambitious goal, researchers and industrialists are working on improving technologies to clean water, with the aim to provide the poorest countries a better chance of access to drinking water.

promising, generating a growing interest and attracting many chemists who try to develop materials on the scale of a millionth of a millimeter for various applications. In order to filter heavy metals and toxins in water, some nanomaterials have been manufactured at a low cost and with little environmental impact. Nanofiltration membranes are widely used: (1) to desalt water, (2) to filter pollutants, and (3) to lower limestone concentration (see *Nature Nanotechnology* 2007).

Nanotechnologies could also provide tools for the detection of pollutants in the air and even to purify it. Volatile organic compounds (VOCs) such as benzene, glycol ether or formaldehyde are known pollutants in the air, particularly in confined areas—habitats, public buildings —, emerging from paint, heaters, air fresheners and even cooking fumes. Chemists are developing nanomaterials based on metal oxides (titanium oxide, platinum) capable of degrading a wide variety of pollutants (VOCs, viruses, carbon monoxide) through oxidation reactions in the presence of oxygen and light (see *L'Actualité Chimique* 2009).

Nanomaterials give rise to many opportunities to be incorporated in materials such as clothes, cosmetics, drugs, tires, etc.; however they raise some questions about their health effects. For water treatment, their high reactivity and small sizes make them difficult to control and they may easily escape into the environment, so that one can wonder if they can damage aquatic life. While many nanotechnologies are still in the research stage, studies and discussions within the scientific community are underway.

### 1.2.2. Towards Cleaner Industrial Processes

In 1998, Paul Anastas and John C. Warner, American chemists from the Environmental Protection Agency (EPA), defined the concept of “green chemistry” as follows: using principles to reduce and eliminate the use or generation of substances harmful to the environment by new clean chemical processes and synthesis routes (Anastas, Warner 1998).

Industrial chemical processes often involve the use of large amounts of organic solvents to dissolve most of the molecules and therefore facilitate their reactions. However they are often volatile, flammable, toxic, and induce some risks, particularly for the operators. In contrast, water is an abundant, cheap, nontoxic, and nonflammable solvent; thus, the development of “chemistry in water” has been encouraged. It is a challenge for chemists since most of the reagents used in syntheses are insoluble or not stable in presence of water. Recent works however show that the use of water for some reactions is possible and can lower

temperatures, therefore economizing energy (Malacria 2008). Ruhrchemie/Rhone-Poulenc process is an example of industrial development using water as reaction medium, annually producing 800,000 tons of valeraldehyde, a chemical intermediate that allows chemists to produce many products such as drugs (Kohlpaintner, Fischer, Cornils 2001). Nevertheless, many industries have also to solve the problems linked with difficult and expensive aqueous effluent treatment.

In general, byproducts of chemical reactions in the industry are a recurring problem as they need to be isolated from the reaction mixture and thus often constitute waste. Therefore, some encourage the development of reactions involving two phases, whether liquid (such as ionic liquids or water), solid (for example with supported catalysts) or vapor to facilitate the purification of mixtures. Solutions are often sought to value byproducts. But a better way is to generate none. In that aim, “click chemistry” is to be considered. It was developed at the beginning of the 21<sup>st</sup> century by the Nobel Prize in Chemistry winner K. Barry Sharpless: these chemical reactions allow us to synthesize molecules very quickly by joining small units together as it often happens in nature (see biomimetics, paragraph 3.1), generating very few byproducts if any, and thus meeting the requirements of the “atom economy” of the green chemistry principles (Sharpless 2001).

Another concern is to avoid long reactions, expensive in energy and dangerous for operators due to important heating or pressure in reactors. In that aim, the use of catalysts is recommended: they speed up reactions and often lower temperatures. They may be also recycled when separation from the reaction medium is possible. “Olefin metathesis” (Noble Prize in Chemistry 2005) is an example of reactions that quickly leads to a wide variety of molecular patterns with little energy and generating little or no byproduct. Many industrial processes are currently using that reaction (Astuc 2004).

Synthesis of complex molecules such as drugs often requires many steps, thus increasing the solvents and energy consumption and decreasing the global yields. The art of “multi-step synthesis” in organic chemistry is changing when passing from the laboratory to the factory. While academic researchers appreciate “elegant” and original syntheses that provide inspiration for their research, simple reactions with low risks of accidents and pollution are rather privileged in the industry. Within the industry, researchers have to consider the criteria, constraints and knowledge of the chemical engineering actors to ensure success when passing from small to large scale, where the behavior of mixtures and the associated effects can dramatically change: for example, while a significant increase in temperature

is considered negligible in a laboratory flask, it can yet become uncontrollable and dangerous in a reactor of several tons.

The researches described above provide only an overview of the many tasks entrusted to scientists, especially chemists, to solve new problems the planet is facing. According to Pierre-Gilles de Gennes, Nobel Prize in Physics winner in 1991: ‘In the elimination of pollutants, the future belongs to chemistry [...]’ (*Les objets fragiles*, 1994).

## **2. What Future for Human Health?**

The topic of health is often closely linked to the questions about the environmental in social debates, since environment directly affects our lifestyle and well being. Chemistry not only helps us to prevent and cure diseases with drugs, treatments and more effective diagnosis, but also plays a prominent role in detecting toxic molecules in the environment and in our food, to track them through our body and to study their transformations and effects on health. In collaboration with other disciplines such as biology, medicine and physics, chemistry has a privileged position in providing solutions to the problems these issues raise.

### **2.1. What Drugs for the Future?**

Drug development is one of the major revolutions of the twentieth century by contributing to increased life expectancy. That would not be possible without major chemical advances which have allowed extraction, purification and characterization of many molecules with therapeutic properties available in nature, and afterward large scale synthesis from various sources (oil, biomass) to make them accessible to the largest possible population. Chemists are even able to imagine novel structures of molecules even more effective than those directly extracted from natural sources. A key to success has undoubtedly been the growing collaboration between chemists and biologists.

The continuation of that collaboration is likely to be crucial for progress in human health research and for the creativity required to develop drugs, vaccines, and gene therapies, but also to design prostheses, artificial hearts, etc. Innovation requires a lot of time of research and development, especially in finding biologically active molecules with fewer side effects. Nowadays, bringing drugs to market is becoming more difficult and expensive. Health and environmental regulations become rightly more and more stringent. The number of molecules entering the

market is globally decreasing from year to year, and health is thereby threatened. Indeed, preserving health may be compared to a race, typically in the case of infectious diseases where bacteria develop more and more defenses against current antibiotics. Tuberculosis is a well-known example of infections resurging in developed countries. In case of failure to eliminate multi-resistant bacteria, infectious epidemics do threaten humanity. Chemists must imperatively find new classes of effective antibiotics, as highlighted by the World Health Organization in 2010.

Yet therapeutic research is likely to benefit in the long run from a major shift driven by recent and unprecedented advances in biology. The new branch of genomics, born in the late twentieth century history through the discovery of DNA, followed by the complete sequencing of the human genome in 2001, is bringing a new view on the living body as a global entity that may be partially controlled by DNA. Thus genomics focus on studying genes and their functions in the body, and by identifying those responsible for precise functions, diseases or genetic predispositions, one hopes to strike directly at the root of diseases, for example through therapies using molecules that would selectively modify gene expression (see EDP Sciences 2010). As more results are found and more phenomena are observed, researchers realize from day to day how complex it is to represent the functioning of the living body: biologists have gradually switched from a simplistic model “one gene for one function in the body” to the observation of crossover phenomena (several genes are involved in multiple functions) as well as parasitic phenomena such as “epigenetic changes”: One realizes that environment and stress may affect gene expression and thereby influence the evolution of an individual life. Chemists and biologists have now to define together the most representative models that could be adapted to complex situations.

The study of genes also opens the way to proteomics, a new science that studies the protein synthesis encoded by genes. Millions of proteins in the body are concerned, including enzymes, the “workers” of the living body. They catalyze many metabolic reactions, but sometimes they can cause some problems that lead to diseases such as cancer, neurodegenerative diseases and many others. In close collaboration with biologists, chemists are seeking to design molecules that interact with the active sites of enzymes, in order to modify their activity and thus suppress diseases. From the three-dimensional structure of an enzyme, chemists are using molecular modeling to test many molecules until they find the one that best fits with the catalytic site structure. They can use the techniques of combinatorial chemistry using robots capable of synthesizing hundreds even thousands of molecules in a short time. These generally small

molecules are then tested on thousands of cells, with the hope of finding a potential drug candidate, able to meet all the pharmacological criteria. Public and private laboratories in the world are now equipped with powerful robots and some make available their databases on the properties of many of the molecules tested. That research field is still in its early days because there is still a vast field of knowledge to explore concerning the functioning of living organisms.

As an illustration, researchers realize that enzymes cannot only be represented by their chemical structure (by the molecular model given by theoretical chemistry), but they evolve in time with their environment: their position in space can be modified by the approach of molecules that will interact with them. Thus, the static model “lock and key” is now switching to a dynamic model that remains unclear. Studies are being led in which chemists design molecules to interact with these enzymes; their interactions are studied through analysis of structural biology, enzymology, biophysics and computer modeling. Answers emerge among others on understanding the mechanism by which a drug could irreversibly bind to its target, so that its effect could be even extended beyond the time of treatment. The understanding of that therapeutic mechanism is likely to generate new research in applied biology (Meinzel, Giglione 2009).

Other major steps are expected and chemists are on the way to better dissect molecular mechanisms in our cells, using improved instruments and new coupling techniques (mass spectrometry coupled with liquid chromatography, etc.). When one progresses in understanding biochemical mechanisms in the body, one gradually moves from research among millions of molecules to verify some rationality in the phenomena of diseases, or even of life.

Today, as time is precious, nature remains an essential guide for chemists. Many pursue the path of designing active molecules from the molecular basis of substances produced by microorganisms, plants, terrestrial or marine animals, and that led to the medicines we know today. Molecules with antibiotic or anticancer activity secreted by marine mollusks and sponges have been recently discovered. There is still an entire world to explore and maybe future new drugs will be provided by the ocean (see EDP Sciences 2009).

In addition, over the past ten years, real hope has been placed in “biomedicines”. These molecules, such as proteins, nucleic acids, etc., are synthesized by methods of combinatorial chemistry or biotechnology. They meet important needs until now imperfectly satisfied by traditional drugs (mainly in anticancer therapy). Their market continues to grow and represents 15% of the therapeutic arsenal in 2012. Another encouraging

aspect is the success rate for researches: three times higher than for “classical medicines”, and sales growth is twice as large: nearly a quarter of “blockbusters” of the pharmaceutical industry (i.e. drugs which generate more than one billion dollars in sales) are now biomedicines (Legrain 2009 and see [www.leem.org](http://www.leem.org)). In that area, many biotechnology SMEs are led to grow in importance, especially in collaboration with big pharmaceutical companies (for example within technopoles), which sometimes also develop their own biotechnology services in close collaboration with their medicinal chemistry services. Another line of research is developing in parallel, in the physical chemistry field of galenics. Effective drugs should avoid rapid degradation in the body and reach their targets quickly and selectively without producing any toxic effects. In that aim, researchers have recently developed systems to encapsulate the active ingredients into nanoparticles whose small size allows them to penetrate into cells. The active molecules are thereby protected from degradation by enzymes, and their pathway through our physiological gates is facilitated to reach precisely the biological targets (e.g. tumors), where the active ingredient is released in a controlled manner and thus reduces the administration dose, decreasing potential side effects. Very encouraging results were obtained, some of which are close to being launched on the market, particularly in the treatment of serious diseases such as liver metastases (see EDP Sciences 2010). Drug research is very emblematic of the growing multidisciplinary collaboration: chemists analyze and understand molecular transformations, biologists elucidate their functions in the body and give to chemists valuable information to find new drugs that they will synthesize with various tools developed by computer scientists, then physical chemists study how to effectively convey drugs into the body. In turn, doctors as well as patients can give their feedback. These multiple collaborations can enhance creativity, which will prove essential for the success of the treatments of tomorrow. On the other hand, to guarantee success, variation of the types of approaches is recommended: preventive or curative, gene therapy, drugs, vaccines, regenerative medicine, etc.

Many countries encourage more and more the development of new ways of organization such as technopoles, associating public and private laboratories of various sizes, such as hospitals and universities, thus gradually moving away from the integrated model of big companies which perform all the stages from the design of molecules to clinical trials. These technopoles can help to promote the dialogue between science and society (including politics), either in the definition of research and development strategies, or in the presentation of scientific work and results.



## 2.2. Materials for Medicine

The therapeutic area also benefits from many advances in the chemical branch devoted to materials. In addition to equipping hospitals with routine care equipment (dressings, gloves, sterile blankets, etc.), that research field is the basis for the design of prostheses, grafts, implants, etc. In that area, the crucial problem of biocompatibility of artificial materials with the human body is often raised: what is biocompatible? Chemists have to use the knowledge of biologists to find ways to deal with defense mechanisms, and also to define with doctors the treatment needs, in order to adapt the shape and lifetime of those materials in collaboration with physicians and bioengineers. Recent discoveries prove once again that collaborations between different disciplines are now a necessity. We can cite here the example of implants based on natural polymers (secreted by bacteria), produced by chemists in the laboratory; the tubes obtained could then repair blood vessels with low risk of rejection thanks to a compatibility with the structure of blood vessels and a well suited elasticity<sup>4</sup> (in *CNRS Le Journal* 2011 pp. 26-29).

## 2.3. Analysis Techniques for Health

Since the late twentieth century, analytical chemistry, as a science and a technology, has evolved both quantitatively and qualitatively. While half a century ago one was measuring milligrams of molecules in environment, food or human body, nowadays one is able to detect traces of nanograms (millionth of milligrams) or even picograms (billionth of milligrams). Thus, a new landscape is emerging which was invisible yesterday and raises today new questions whose answers still generate more! Now doctors, chemists and biologists are even able to see live on a computer screen what happens in a living body without making any incision.

### 2.3.1. Analysis and Medical Imaging

For the last thirty years, powerful and non-invasive imaging techniques have been developed to observe organs and tissues, allowing doctors to detect earlier abnormalities (such as tumors, stenosis of blood vessels), locate them precisely, evaluate their progression and diagnose earlier and

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<sup>4</sup> It should be noted that the works cited are by the team of Didier Letourneur, who is all together a chemist, a biologist and a physician. Further work on the bone implants have been successfully completed by a laboratory in Nantes, in a unit named "Chemistry and Interdisciplinarity".

earlier. Magnetic resonance imaging (MRI) is one of these useful techniques. To improve image quality, contrast agents can be injected into the patient's body. Those are molecules developed by chemists whose paramagnetic properties can amplify the signal in regions where they are located, thus amplifying the image contrast. A current path of research and development consists on applying magnetic resonance imaging at cellular or subcellular level. That can allow doctors to visualize non-invasively many processes taking place on that scale by imaging the evolution of molecules in the body, such as the consumption of glucose by cancer cells. One can also follow the activity of macrophages associated with multiple sclerosis, the accumulation of beta-amyloid plaques in Alzheimer's disease, or even the consumption of folic acid by tumors of ovarian cancer. Many advances have been made in that very new area of research that should also help to better understand the functioning of the body, to follow the evolution of a drug or other xenobiotics, and even to understand phenomena still poorly understood such as the aging process (see EDP Sciences 2010).

### **2.3.2. Toxicology as a Growing Research Field**

Environment and health areas benefit from finer and finer techniques in chemical analysis that have been becoming valuable allies to track down the smallest traces of pollutants and toxins. It is an indispensable tool for the implementation of standards and regulations to protect our health. Yet, how to set these standards in a meaningful way? Toxicology is a developing research field devoted to studying the effects of exposure to substances both with the body and the environment, by studying the ways to detect them. For a given molecule and dose, the nature and effects of the poisoning severity and their speed of onset (acute or chronic) are measured. Toxicologists are still facing many issues: how to define toxicity thresholds for molecules that are always mixed with other pollutants? How to account for individual differences in sensitivity and for delayed onset of symptoms over time? Recent advances are nevertheless important and many studies are designed to model the effects of toxins, to find biomarkers in order to monitor the evolution of molecules in the body, etc.

These works involve an increasing pluridisciplinary collaboration mobilizing biology, pharmacology, physical chemistry, statistics, and epidemiology in response to growing societal needs. For example, chemical industries must appeal to pharmacologists to help evaluate the toxicity of their products in the context of REACH.

We realize how major scientific discoveries since the last century have impacted chemists' practices, and new branches have appeared: genomics, nanoscience. Scientists are now able to go further in the invisible, the infinitely small, the infinitely fast, often without causing damage to the environment, whether matter, nature or humans. Predictive tools are becoming more used. It is now possible to collect in a short time impressive amounts of results with the help of computers, which can also accelerate the flow of information between scientists. In the same time with the evolution of chemistry in response to environmental and human challenges, its relationship with environment and society is also evolving.

### **3. What Chemistry for the Future Society?**

#### **3.1. Chemistry in Complex Environments and Contexts**

Through these environmental and human issues, chemistry is appearing everywhere: whatever the scale (from carbon nanotubes to carbon cycle), whatever the environment (land, sea, air, space, human body, plants and laboratories), chemical knowledge is used. However, molecules and materials in the world always interact with complex environments where their various properties (chemical, physical, biological) emerge and also evolve in complex ways. How to study these environments, how to rationalize them? Are chemical and computer models relevant enough when they mimic the living body and nature? How far can we rely on them to make decisions that may impact our health and the environment? That question is raised in the context of REACH regulations, which limit toxicity tests on animals. Therefore researchers have to find the most representative models, whether cellular or computer. The next issue will be how to test these models in real-world experiences, that is, people's living environments, and to define the way to rectify these models appropriately when necessary.

Sharing continuous reflections with other scientific disciplines is proving indispensable, especially when a molecule or a concept in a laboratory is brought into contact with citizens and societies, with economic and human realities. Each actor in the chain has to consider the criteria of the beliefs and welfare, the rights and duties of the others, as well as the outcome in the end of the chain, and chemists themselves cannot ignore other chemists (for example researchers/engineers), otherwise formal application of "principles of green chemistry" would no longer make sense: is it enough to do chemistry in water for sustainable development? Is it enough to use renewable resources? Does

biodegradability always ensure protection of the environment? After all, how to do sustainable development? An interesting example of chemical process that tries to “get closer to nature” is “biomimetic chemistry”, which is attracting more and more researchers. Natural processes that have developed over millions of years of evolution are remarkably optimized to allow animals and plants to live in harmony within ecosystems. The best-known example is photosynthesis, which uses environmental resources (carbon dioxide) while consuming minimal solar power: one can see it as a model of sustainable development. Thus research laboratories are working on developments inspired by natural processes such as dye sensitized solar panels for better photovoltaic yields (inspired by photosynthesis) (Lincot 2011), chemical reagents mimicking nitrogenases (clover and alfalfa enzymes involved in the production of ammonia) to produce nitrogen fertilizer with little energy (Le Goff 2010), and many other examples. In each case, the question should be asked again: how can biomimetics help sustainable development? At least, it leads on to be conceptually closer to nature, but that is another goal.

It is clear that the reflections must be collective and each case is unique, depending on complex global contexts in continuous evolution, and at any time foundations of formalisms have to be re-examined in confrontation with real-world experiences.

### 3.2. Meditating about Chemical Applications

As discussed, the choice of resources and processes in industrial developments is a complex issue. On the other hand, the purposes of developments and the choice between doing or not doing something are yet another concern. Here again, the need for reflection does not only belong to chemists but to all of us. For example what path to take to provide taxol<sup>®</sup>, the anticancer substance present in the bark of the yew tree, which is a slow growing tree<sup>5</sup>? Was it necessary to sacrifice or give up forests to save lives? Moreover, bringing a drug to market raises the question of the balance between benefit and risk: to what point should innovation be pursued or held back? If one pushes the thinking in its own terms: what is an acceptable risk, and after all, what does progress mean<sup>6</sup>? On the other hand, what are the limitations of human intervention? To

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<sup>5</sup> That question was solved in the 1980s with a synthesis of Taxol<sup>®</sup> and Taxotere<sup>®</sup> (a derivative even more active) from the thorns of the European yew *Taxus baccata* by Prof. P. Potier' team (France).

<sup>6</sup> The question was discussed at the 3<sup>rd</sup> forum “Science, recherche et société”, June 16 th, 2011, Collège de France (Paris). Organized by *La Recherche* and *Le Monde*.

what extent are we able to predict the long-term consequences of human activities? Could we predict the magnitude of the problems associated with greenhouse gas emissions at the industrial revolution period? Can we predict and control early enough any risk of drift due to discoveries and developments?

Chemists do not control all the possible impacts of their discoveries and developments, however they can at least try to master the understanding of the objects they create, being conscious of the fact that their understanding can meet some limits. With that knowledge they must then occupy a significant place in substantive discussions involving other actors of the society: politicians, economists, sociologists, philosophers, and historians, to reflect on the importance and directions to give to research and developments, while weighing the risks and the benefits.

Beyond the balance of risk/benefit, a fundamental question is emerging: “what kind of society do we want to build, on what basis and on what values?” Understanding, manipulating and creating matter is never neutral and integrates into a human culture, as diverse as it is, as contradictory as it can be. Chemistry and its activities cannot be isolated from social debates.

### **3.3. Towards New Relations between Chemistry and Society**

Nowadays, researchers and industrial chemists sometimes face contradictory situations, particularly in France: on the one hand, society expects them to find quickly solutions to the resource and energy scarcity, and the “zero risk” criterion for consumer products is required in developed countries. On the other hand, research is not always encouraged and some scientists even face hostile behaviors (studies on GMOs prevented, debates on nanotechnology in 2010 sabotaged).

To ensure their role in our daily lives and to face contemporary challenges, chemists are required to develop a sustainable relationship with society. They particularly need encouragement and support from political leaders, who are sensitive to public opinion, because the entire society ultimately uses the objects and tools created through chemistry. They also need illumination from social sciences to understand how society can accept their science in its current logic and practice, or conversely, how chemistry can be adapted to the nature of contemporary societies.

In order to be understood, chemists communicate more, especially since the media have multiplied. Researchers, industrialists, scientists, teachers and mediators have multiple opportunities to convey a positive

image of chemistry through lectures, books, television and radio, exhibitions and practical experiences such as those in the operation *La main à la pâte*<sup>7</sup>. One can thus excite the public or simply make the activities of scientists and engineers more accessible in order to gradually break down the frontiers between science and the public. That is encouraged by the Roberval Prize in France since 1986 to reward works (books, TV shows, software, websites) bringing to the attention of the public news and technological knowledge, e.g. on *Nanotechnology and Health*, developed on a website awarded in 2008<sup>8</sup>. For the researchers, the concern to make the public understand their activities is growing, as evidenced by the establishment in 1995 of the “Centre de Vulgarisation de la Connaissance” at the University of Orsay in France, leading researchers to explain their research to the public, for example in an interview. That raises some questions: what message should be transmitted? What is the public really expecting, consciously or unconsciously? How can sociology, psychology and cognitive sciences help researchers to enter in contact with that very diverse public?

Overall the image of chemistry to the public has obviously evolved with the media. Emissions, reports and films demystify chemists and show them active in the field: they take part in police investigation, restore and authenticate artworks, take samples from archaeological excavations as well as from the ocean depths, control doping in sports competitions, detect food fraud, etc.

By other means, efforts are made to show that chemistry is useful and to encourage the younger generation to engage in a forward-looking branch<sup>9</sup>. Thus the new science curricula of French high schools since 2012 are based on a thematic approach to science: among the titles, “contemporary global issues” appears; a second theme concerns the importance of soil and water for agriculture and therefore the challenge of

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<sup>7</sup> The operation *La main à la pâte* was launched in 1996 at the initiative of Nobel Prize in Physics 1992 Georges Charpak, Pierre Léna and Yves Quéré and the Academy of Sciences, and is extended at international level: in hands-on sessions teachers submit to the curiosity of students from primary school objects and phenomena of the world around them, creating scientific inquiry. This led to the formulation of hypotheses intended to be tested by experiment or verified by a literature search. Thus, students gradually take ownership of scientific concepts and operative techniques and strengthen their oral and written expression. [www.lamap.fr](http://www.lamap.fr)

<sup>8</sup> <http://www.cnrs.fr/cw/dossiers/dosnano/>

<sup>9</sup> See the symposium “Enseignement de la chimie pour un développement industriel durable”, septembre 5<sup>th</sup> 2011, organized by Société Chimique de France ([www.societechimiquedefrance.fr](http://www.societechimiquedefrance.fr)).

feeding nine billion people. Teaching chemistry through concrete thematic also helps young people to better visualize careers in chemistry. The underlying question is how to inform and motivate them in the long term. The future questions will be: what relationship will they have with chemistry tomorrow, and with science in general; how will they build these sciences and how will they integrate their past, their history, in the context of a globalized world with its culture(s)?

### **Conclusion: The Challenges of Chemical Practices go Further than Chemistry**

Chemistry is definitely a key player for the future of humanity among other main scientific disciplines with which it is increasingly collaborating. As a theoretical science, it is essential to better understand natural phenomena, from the cell to the planetary scale, and to play the role of expert to guide us in our business and political choices.

As an applied science, chemistry is a major innovation actor needed to find solutions to resource scarcity, develop renewable energies, find new drugs, manufacture recyclable materials and insulation materials to conserve heat, synthesize fertilizers with respect for the environment, etc. Recognizing that vital role to meet global needs, Ethiopia suggested that 2011 should be an International Year of chemistry. That was then proclaimed by the United Nations.

Today chemists' work is oriented by an extreme pressure: they are more than ever driven to a responsible attitude in the implementation of production processes, they must both strive for zero risk and continue progress, taking into account economic, political, social and demographic factors which accompany the development of a truly sustainable development, which is thus not only a scientific issue. That equation is the most difficult they have ever had to balance and its dynamics are so unstable in an unstable world!

As actors of the society, chemists must also participate in collective reflections on the choice of priorities to be adopted in each country: according to the majority demands, the economical needs, or according to a scale of value to be defined? Can we put the same level of urgency to feed hungry people and to provide to others fuel to travel? These ideas are firmly part of the spirit of sustainable development. Reflections are always difficult because one must take into account individuals' sensitivities and values. Moreover, societies may accept or reject technological developments. Indeed the whole society, inserted into the global world, is building its future. How will chemistry, as it has been built, succeed its

long-term integration in the new world? One of the prerequisites will probably be to build a trusting relationship. For that, all actors in the society have a role to play, at all levels and in the wider context, whether scientists, politicians, historians, social scientists, teachers, parents, or ordinary people. In all cases, some progress in that globalized world will not go without new difficulties, neither without generating more anxieties among populations for whom changes can go too fast and affect confidence. Maybe there is a price to pay and a courageous, creative and hopefully mind to seek, with the aim of preserving our future, thinking of the future generations.

Ultimately, the role of chemists should be constant in the past as in the future, that is, doing their job with awareness, adapting to the world, learning from past mistakes, and in fact being citizens of the planet.

After all, can chemists only say what it means, according to them, *to be a chemist*? Is it mostly a question of knowledge, tools, methods, techniques, position in a community or a society, practices, mind, art, values, heart? Does chemistry have a precise and deep identity, while being able to open itself to other disciplines and actors?

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# LIFE CYCLE ASSESSMENT AND ECODESIGN: INNOVATION TOOLS FOR A SUSTAINABLE AND INDUSTRIAL CHEMISTRY

SYLVAIN CAILLOL

## 1. Context

### 1.1. The Chemical Industry Mobilized to Global Turmoil

Our society became recently aware-on the scale of humanity-that it was mortgaging its collective future to meet its need for individual wealth. As long as we were only a few hundred million people on Earth to share the most of the wealth and generate, consequently, most of anthropogenic pollution, the balance-questionable, certainly-was maintained. But with the arrival in the last decades of nearly 3 billion people, Indians, Chinese, who claim-rightfully so-a high level of consumption, and with the prospective increase of the world's population in the forthcoming years, the international community calls for sustainable development to establish a new truly sustainable balance.

Thus, the 20<sup>th</sup> century has been marked by unprecedented population growth, economic development and environmental changes. From 1900 to 2000, the world's population grew from 1.6 billion to 6.1 billion people. However, as the world's population quadrupled, the global real GDP increased from 20 to 40 times, thereby allowing the world not only to withstand a quadrupling of the population, but also to do so under significantly higher conditions of life. Nevertheless, this population increased and this rapid economic growth was uneven across all countries, and all regions also did not equally benefit from the economic growth. In addition, population growth and economic development, which occurred simultaneously, led to increasing unsustainable use of the Earth's physical environment.

The analysis of interrelationships among the population, environment and economic development is much older than that of Thomas Malthus (late 18<sup>th</sup> century). Indeed, since ancient times, statesmen and philosophers

have been giving their views on issues such as the optimal number of the population and the disadvantages of excessive population growth. Thus Plato and especially Aristotle fed many thoughts on the balance between population and natural resources, defined as livelihoods and, more specifically, food and water. These thoughts were also carried out by Montesquieu in the 18<sup>th</sup> century. And the activity that the United Nations devoted to population, environment and development is as old as the Organization itself.

In the 1960s, we became more and more aware that the world population growth had reached unprecedented levels; a situation considered seriously worrying in many studies and debates. A report of the Secretary-General entitled "Problems of the human environment" mentioned "explosive growth of human populations" as one of the signs of a global crisis concerning the relationships between man and his environment. This report was an essential milestone of the process that led the United Nations to convene the United Nations Conference on the environment held in Stockholm in June 1972. This was the first global Intergovernmental Conference devoted to environmental protection. The 20<sup>th</sup> century has been marked by an extraordinary increase in the world population from 1.6 billion to 6.1 billion, 80% of which occurred after 1950. And the world's population should continue to grow. On the basis of varying fertility average, the United Nations expects the global population to reach 9 billion by 2043 and 9.3 billion by 2050. However, small but steady deviations of fertility rates can influence the size of the population over time. Thus, scenario of high fertility in which the fertility rate is higher than half a child to the average fertility scenario, provides a size of 10.9 billion people by 2050.

Urbanization is another important trend. Indeed, although the world population may double in the next 40 years, the urban population, now of 3 billion people, is expected to double with energy needs that will also increase considerably. Among these "neo-urban", by 2050, will be also nearly 1 billion climate refugees, driven by large mining or dams projects, and by the effects of global warming and conflicts inherent to the generated changes.

This expected population growth in the forthcoming years will also be accompanied by an increase in individual consumption. The first item of consumption will be energy. International Energy Agency IEA estimates lead us to imagine several worrying scenarios that might arise by 2030: a doubling of energy demand compared to the 11Gtep (gigatons of energy of oil equivalent, or 11 billion tons of oil-1 ton of oil corresponds to 41, 9GJ) consumed in 2007! If this evolution occurred, it would result in a doubling

of the emissions of CO<sub>2</sub>, the main greenhouse gas! At the same time, the growth of the population would require a doubling of agricultural production to meet its food needs by 2050. But our Earth's resources are limited and some begin to miss. Indeed, the last two reports of the "Joint Operating Environment"-JOE-on "environment" of US Joint Forces occupy an important place among recent analyses that recognize the possibility of a fall in global oil extraction by the middle of this decade. Indeed, these studies report in identical terms a diagnosis that figures among the most pessimistic on the question of a possible structural oil shock by 2015: 'in 2012, surplus oil production capacity could entirely disappear, and by 2015, the production deficit would be close to 10 million barrels per day', equivalent to the daily extractions of Saudi Arabia. The 2010 report of the IEA shows that almost 30% of the production of active wells today will be extinct within 10 years, decreasing from 68 to 48 million barrels per day (mb/d) by 2020. And within a generation, by 2035, currently operated oil fields would provide less than 17 mb/d, which corresponds to less than one-fifth of future demand. Even if new resources are found (oil sands, shale gas, etc.), their price will be a critical issue. Indeed, based on their price we can afford or not energy production and consumer goods. Other non-carbon resources are also in exhaustion, such as terbium, hafnium or silver deposits that could be exhausted (for operations at a reasonable cost) respectively by 2012, 2018 and 2021-2037. Thus, we can update the famous sentence of Paul Valéry (1945) "the time of a finite world begins"-we are testing it every day.

## **1.2. The New Constraints on Industrial Chemistry**

Our society is currently based on the almost exclusive use of fossil resources, especially for energy supply and consumer goods. The question is not whether or not there will be production peaks, but rather *when* these peaks will occur. Indeed, almost all experts agree on the amount and duration of our global reserves of oil, coal, gas, uranium... based on our current consumption rate. Thus, at the end of this century, we will have exhausted all the land reserves that nature has taken millions of years to form. However this exploitation of fossil fuel resources-fossil carbon-is accompanied by a transfer of carbon, which by combustion occurs as CO<sub>2</sub> from fossil origin in our atmosphere, accumulates, and contributes to increase the concentration of the famous "greenhouse gases", responsible for the rise in average global temperatures.

These issues are the new constraints of industry and in particular of chemical industry—the industry of industries—since more than two-thirds of its products are intended for downstream industries. And because of these constraints, chemical industry will undergo a revolution based on:

- The anticipation of exhaustion of raw material coming from fossil resources with higher price volatility. And the unequal distribution of these fossil resources, especially oil, gives rise to significant speculations that jeopardize a stable supply.
- An obligation of drastic reduction in the emissions of chemical processes and in particular the release of greenhouse gases (CO<sub>2</sub>, NO<sub>x</sub>). The evolution and the level of supply of fossil fuels increased considerably the quantities of fossil CO<sub>2</sub> emitted each year into the atmosphere. Chemistry is relatively low emitting CO<sub>2</sub>, but it is very sought to identify new processes to reduce emissions of CO<sub>2</sub> of energetic origin, store CO<sub>2</sub> or value it by remediation (use as input<sup>1</sup>).
- A strong regulatory pressure on toxicology and ecotoxicology related to the use of raw materials, of synthesis intermediates and chemical industry products, including REACH regulation, the framework directive on water FDW, but also to numerous European directives about the end of life of the materials (end-of-life vehicles EOLV, waste electrical and electronic equipment WEEE, directive on volatile organic compounds VOC emitted by varnishes, paint and refinishing of vehicles, etc.).

If the first regulations on industrial activities date back to 1810 with a Napoleonic decree that was requiring compliance with a distance around production sites, the first European directive controlling the toxicity of chemical production was established in 1967 with the directive 67/548/EC on the “classification, packaging, and labeling of dangerous substances”. Since then, the number of European directives related to the environment has increased dramatically, particularly since the late 1990s. All of these regulations are severe constraints for the chemical industry but may turn out to be stepping-stones for innovation.

Thus, covering the needs of humanity (food, energy, and health) while respecting our environment is the challenge awaiting us, and which chemistry will have to face in the forthcoming years. Chemistry has already managed to win battles in the last century—fight against epidemics, agricultural increase, agri-food and industrial productivity to meet the growing demands for food and consumer goods, etc. **Currently the**

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<sup>1</sup> Input: Element that enters into a production process.

**demand is different, but it is still chemistry that has the keys to sustainable development.** Indeed, chemistry, on a strict etymological perspective, is the science, the art of the Earth. Therefore it is chemistry that is sought to address these challenges as a science but also as an industry since chemistry is at an upstream position with regards to all other industries (60% of the production of chemical industry returns to industry<sup>2</sup>). Chemistry is at the heart of the production process, but it can take only the choices and decisions relating to arbitrations concerning production processes and resources, in particular with a view to reduction of environmental impacts. Life cycle assessment can be a tool to justify these choices. But in all cases, we will see that the choice may be made only after interpretation of the results of an LCA. Chemists, biologists, and toxicologists are indeed asked for the interpretation of the results of impacts. But on the basis of what criteria should we make these choices? Prioritizing what expectations? It is perhaps in this interpretation that we demand an inspired enlightenment from philosophers and historians.

## 2. Life Cycle Assessment, Tool of Ecodesign: Definitions and Concepts

### 2.1. Ecodesign: Some Definitions

The productions of goods and service are now under stress. It will no longer be sufficient to meet the specifications by technical means in accordance with the cost limits; we will also have to integrate the respect for the human and the environment, which means reducing the consumption of fossil resources, limiting greenhouse gas emissions, complying with the environmental constraints—this amounts to **limiting environmental impacts**. But taking into account all environmental impacts during the manufacturing process, and not only the measurement of the carbon footprint or CO<sub>2</sub> emissions, amounts to the integration of **ecodesign** to the conventional design process, and also consequently to the innovation processes. This innovation process undergoes significant changes. We do not expect a quick response but a time for reflection is allowed to provide a comprehensive answer on the environment, an “ecodesigned” answer.

Moreover, ecodesign is part of the recommendations of the “Grenelle Environment” forum held in 2007. Indeed, the commitment n° 217 encourages environmental analysis approaches of products and ecodesign:

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<sup>2</sup> Please refer to: “UIC, Bilan de l’industrie chimique en France, 2008.”

Commitment n° 217: to generalize the environmental information on products and services: label energy applied to the whole of products high consumers of energy, with a single referential; development of eco-labels; accompaniment of voluntary efforts on the implementation of information on environmental impacts, with progressive obligation to provide this information; review of the generalization of the ecological price (double price to inform the consumer of the impact on the environment of property purchase) from term to a collaborative eco-contribution.

Finally, the ecodesign is from now a regulatory obligation with the framework directive for Ecodesign (Energy Using Product EuP) that states, for energy consuming products, that: ‘the ecodesign of products is an essential axis of the Community strategy on integrated product policy. As a preventive approach, designed to optimize the environmental performance of products while maintaining their quality of use, it presents new and real opportunities for manufacturers, consumers and society as a whole’. This directive has been reinforced by another directive laying down ecodesign requirements for the following products: hot water boilers with liquid or gaseous fuels, refrigerators, freezers and combined appliances to household use and ballasts for fluorescent lighting. Ecodesign therefore begins to become an obligation. It is also a response to consumers’ expectations. In fact, end-users are now waiting for eco-friendly products. Indeed, according to the IRSN<sup>3</sup> barometer, since 2006, the degradation of the environment is in the top 3 concerns of the French people.

Ecodesign is a comprehensive approach, which is focused on the product. It mainly takes into account human and environmental criteria from the design phase of a product. These criteria generally relate to all the steps followed by a product, production, distribution, use and end of life, namely: the **life cycle** of a product (cf.—Figure 1). Ecodesign is a multicriteria preventive process, which seeks to identify and reduce at the source all impacts on the environment.

The concept of eco-design is based on a powerful tool to identify the environmental impacts: the life cycle assessment LCA.

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<sup>3</sup> The IRSN is a public organization, expert in research and expertise on nuclear and radiological risks.

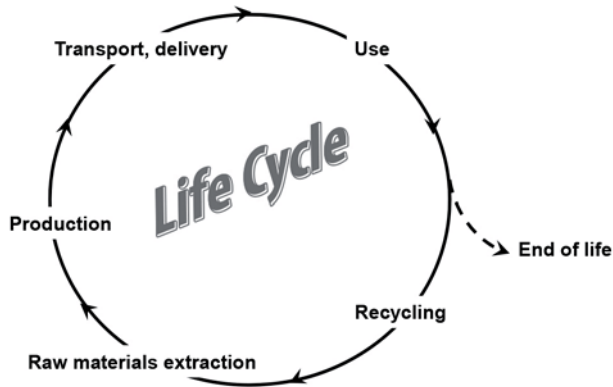


Figure 1: Life cycle of a product

## 2.2. Life cycle Assessment: History

Life cycle assessment, as practiced, is actually an environmental life cycle assessment as the evaluated impacts are mainly environmental impacts.

The “life-cycle assessment” thinking is a holistic way of thinking, which takes into account all impacts, environmental, social, and economic on the whole life cycle of the product or service. This way of thinking should help to prevent local improvements from resulting into a transfer of problems (pollution, social conditions, etc.).

LCA dates back to the late 1960s and to the early environmental assessments conducted in the USA on the REPA-Resource and Environment Profile Analysis-model. These assessments aimed to compare materials for packaging applications and focused on the energy consumption, consumption of raw materials, natural resources, and waste production, in relation to the discussions of the moment on growth and environment (Club of Rome). In the early 1970s, following the first oil shock, industrial companies were essentially doing the inventory of energy flows consumed by their activities, under the form of analysis of environmental profiles, and use of resources, at the expense of real environmental analyses. In the late 1980s a renewed interest emerged for environmental analyses, in relation to the problems of solid waste. Matter and energy inventories were also used for *marketing* purposes. The initial methods led to results that were difficult to use from one country to another, and from one product to another, because of the heterogeneity of the data used and the



various approaches. Industry and government had called for the development of a systematic, repeatable and comparable methodology at least on regional scales. The SETAC (Society of Environmental Toxicology and Chemistry) and the BUWAL (Switzerland Department of the Environment) had then responded to this call and the first Swiss method of environmental analysis of BUWAL appeared in 1984.

The concept of **life cycle assessment** appeared truly for the first time during a seminar in Vermont (USA) of SETAC in 1990, which focused on the need to extend the environmental analysis based on material/energy balance to a real life-cycle assessment-the concept of impact assessment was established. The first life cycle assessment was therefore carried out in France on the steel packaging products of SOLLAC Company. In 1993, SETAC proposed a code of good practice, which constituted the reference frame for future developments. In 1997, the ISO-International Standard Organization-published the first international standard on life cycle assessment-ISO 14040: Environmental Management-life cycle assessment-principles and framework. In 1998, ISO published the international standard ISO 14041: Environmental Management-life cycle assessment-definition of the purpose and the field of study and analysis of the inventory. In 2000, the ISO published the international standard ISO 14042: Environmental Management-life cycle assessment-life cycle impact assessment, and the international standard ISO 14043: Environmental Management-life cycle assessment-interpretation of the life cycle. LCAs were developed in France in the 2000s with the handling of LCA by specialized firms and in 2005 the organization of the first Symposium on Ecodesign and Chemistry in France by the French Federation of chemistry FFC and ChemSuD<sup>4</sup>. In 2006, the ISO published the standard 14044: Environmental Management-life cycle assessment-requirements and guidelines and established a new version of the 14040 standard. These two new standards cancelled and replaced the previous standards ISO 14040 14041, 14042, 14043.

### 2.3. Life Cycle Assessment: Definitions and Concept

Life cycle assessment is an analytical method, which consists to quantitatively evaluate all of the potential environmental impacts of a product or service by considering the entire life cycle.

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<sup>4</sup> ChemSuD Chemistry for Sustainable Development–European Chair based at Montpellier Chemistry School.

This analysis can be applied to the entire life cycle, in a “from the cradle to the grave” approach, to the extent that at each stage of the life cycle there is consumption of energy and resources, and generation of environmental, social, and economic impacts.

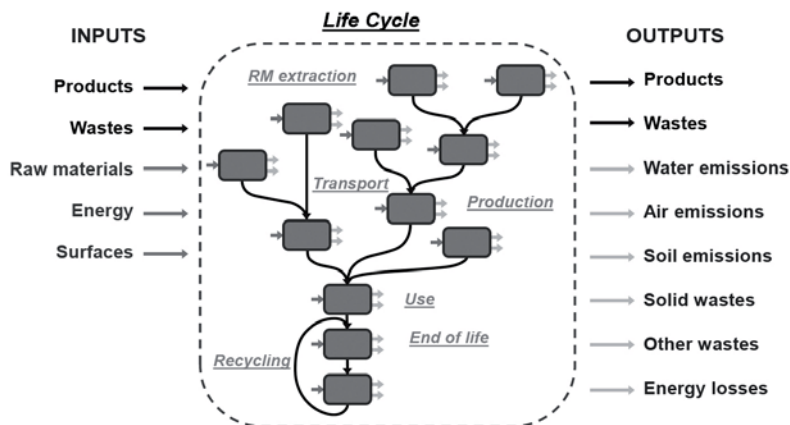


Figure 2: LCA principle<sup>5</sup>

Life cycle assessment therefore consists in evaluating, within a system defined by some limits, the impacts due to **inputs**—consumption of natural resources—and **outputs**—emissions into air, soil, water, and other nuisances (cf. Figure 2).

This analysis is actually based on four well-defined phases: the **definition of objectives** and the framework of the life cycle assessment; life cycle **inventory**, the **evaluation of the impacts** of life cycle, and finally the **interpretation** of the life cycle. The analysis is based on a scientific methodology, which relies on computer software, supervised by the ISO standards 14040 and 14044.

## 2.4. Definition of the Objectives and Framework of Life Cycle Assessment

The definition of objectives and the scope of the life cycle assessment is the subject of a reference document, which is updated at each stage of the assessment. Generally, the life cycle assessment studies are conducted

<sup>5</sup> Document originates from the author.

in order to answer specific questions regarding environmental impacts by comparing different products or services. In all cases, these are comparative analyses that are **attributional**. They can be made to answer issues related to the consequences of the massification of a process-for example the consequences of the generalization of a limited or localized behavior: in this case there are **consequential** life cycle analyses.

To define the **objectives** of the study, the intended application should be specified, and the reasons leading to conduct this study and the public concerned, namely those to whom it is intended to communicate the results of the study, should be defined. Secondly, we should define the **scope of the study** that enables us to restrict the study to the given *limits* and to establish the limits of the system studied, to define the activities and impacts that are included or excluded from the study. We define the *temporal* cover (system lifespan), the *geographical* cover, the *technology* cover, the cover of the *processes* (system boundaries), the cover of *environmental interventions* (inputs and outputs), and the cover of the *potential impacts*.

A list of environmental references may be used in order to determine the impacts related to the ongoing project. The study of this list will help us to eliminate unnecessary impacts categories, to arrange the categories with insignificant impacts at a low level of analysis and thus to identify the critical impacts. This amounts to setting an *inclusion threshold* for the impacts on life cycle assessment.

*Inclusion Threshold:* it is generally impossible to take into account all the compounds forming a complex product. The head of the LCA is therefore required to establish an inclusion threshold, corresponding to *negligibility* rules which principle is as follows: all components representing less than X % of the total mass of the product are neglected. Secondly, we verify that the sum of what is taken into account remains above a fixed percentage, which is always close to 100% and, qualitatively, that the neglected compounds are not characteristics of particular danger (ex: toxic substances, radioactive waste) or other established specific problems (ex: production process known as a particularly polluting or consumer of energy). If not, these compounds will be reintegrated into the analysis, whatever their quantity may be.

The definition of the system also includes the definition of the *functional unit* and that of the *reference flow*.

The functional unit is a quantity, which allows one to quantify the function of the studied system and to compare different systems performing the same function.

*Examples:*

- *In case of an LCA to evaluate different packaging, the function studied is packaging. The functional unit to be defined is therefore a packed volume  $V$  (in  $m^3$ ) and not a packed mass (kg) or a mass of packaging materials.*
- *If the analysis focuses on the comparison of processes of waste treatment (storage, incineration, recycling), the functional unit may be for example, the treatment of one ton of wastes.*

This definition phase is really crucial, as the results of LCA depend greatly on the objectives and framework that have been previously set (but normally neither the sponsor nor operator). Thus, the LCA of a plastic yoghurt pot from a particular manufacturer, knowing accurately the transport distances of their products as well as the composition and the different modes of energy production that are used, will not give the same results as the LCA of the European yoghurt pot, conducted on the basis of average European production. Therefore, to avoid inaccurate interpretations or generalizations in the use of results, the objective and scope of the study should clearly explain the studied issue.

## 2.5. Life Cycle Inventory Analysis

This phase is the one that was the most developed at the methodological level. It benefited from methods coming from raw materials/energy balances of the 1970s. The definition of the life cycle inventory analysis according to international standards is: "Phase of the analysis of life cycle involving the compilation and quantification of the inputs and outputs for a given system of products in its life cycle". The inventory is the basic objective of the LCA, as it is constituted by the basic processes that obey the physical laws of conservation of mass and energy. However, this type of inventory is not absolute. Indeed, this approach involves a phase of data collection related to the achievement of working hypotheses. The data can be collected not only on production sites but also with complete data from trade associations or organizations.

It consists here to collect data or gather existing data, and make the calculations according to a specific workflow: the flow chart, description of each basic process, and data validation. The quantitative input and output data of each elementary process calculated with respect to the reference flow are put in relation to the functional unit.

All environmental interventions (use of resources and emissions of pollutants) for the system of products for each unitary process at each stage of the life cycle are thus summed into an inventory table and

expressed with respect to the system reference flow. At this point, during this aggregation, the spatial characteristics (place of emission) and temporal characteristics (time of emission) are generally lost. This may be harmful to the actions to be taken after a life cycle assessment in so far as the inventory is very spatialized in our global economy (example: production of oil in the Middle East, refining in the United States, production of intermediates for synthesis in Europe, production of ores in Asia) and also registered in time as technologies change rapidly and as a result their environmental impacts.

The inventory data are composed of material flows (minerals, iron, water) and energy (oil, gas, coal), entering the system under study and of the corresponding outflows (solid waste, emissions gaseous or liquid). There are some life cycle inventory databases especially for common raw materials, energy, and transport. These data are available at low cost in the form of public or published databases (example: *Ecoinvent* database of “Swiss Centre for Life Cycle Inventories”).

Some groups or professional federations have also collected data on the environmental impacts of their material throughout the life cycle or, more frequently, on the upstream part of the cycle to make them available to the users of such materials so that they incorporate them into their own LCA. For specific data related to a given study, data collection has often to be carried out on an individual basis, for a collection on industrial site through bibliographic research, or through the perspective of previous studies.

Case of plastics: the APME (Association of Plastic Manufacturers in Europe) provides for free by mail and on its website the “ecoprofiles” of major plastics, in the form of lists of averaged inventory results which are easily usable in spreadsheet or calculation software.

## 2.6. Evaluation of the Impact of Life Cycle

The *impact assessment* phase consists in explaining and interpreting the results obtained during the inventory, in terms of impacts on the environment, and in the form of an adequate summary that could be understood by a non-specialist. This phase should help to prepare the disclosure of elements related to the product environmental impact. It is particularly sensitive.

The two previous phases-*inventory* and *assessment*-are those that are more related to chemistry insofar as the entire process of manufacture is decomposed into mass balance and energy balance and is divided into primary inputs: oil, gas, etc. Each step of this process, by-products, and

effluents are identified and their fate is assessed in terms of possible direct or indirect pollution. To conduct the impact assessment phase: (1) *impacts categories must be selected* (cf.

Figure 3 below), (2) *impacts indicators* and characterization models *must be defined*, (3) and the *allocation of inventory results* should be achieved in the different impacts categories (*classification*). For each indicator category, we must calculate the results (*characterization*), the amplitude of the results in comparison to references values (*normalization*), the grouping and ranking of indicators and the *weighting* of indicators.

Basis categories of impacts	Complementary categories of impacts
<b>Depletion of abiotic resources</b>	Loss of biodiversity
<b>Land occupation</b>	Ionizing irradiations
<b>Climate change</b>	Odors
<b>Destruction of stratospheric Ozone layer</b>	Noises
<b>Human toxicity</b>	Drying
<b>Ecotoxicity</b>	
<b>Photo-oxidative pollution</b>	
<b>Acidification</b>	
<b>Eutrophication</b>	

Figure 3: Impacts categories<sup>6</sup>

The impact indicators rely on various methods, which come from various sources.

*Example: For an inventory result that identifies the release of various compounds such as cadmium, CO<sub>2</sub>, NO<sub>x</sub>, SO<sub>2</sub>, etc., acidification will be defined as one of the impact categories. In this case, the inventory outcome allocated to the selected impact category includes acidifying emissions due to NO<sub>x</sub> and SO<sub>2</sub>. Modeling of the category indicator is the*

<sup>6</sup> This document originates from the author.

*release of proton  $H^+$ . The chosen indicator is aggregated to an acidification potential AP expressed with  $SO_2$  equivalent unit. For the aggregation, weighting coefficients are the following: 1 for emissions of  $SO_2$  and 0.7 for emissions of  $NO_x$ . On the point of application of category, it is composed of ecosystems such as forests and vegetation*

It is imperative that the chosen indicator provides an appropriate representation, namely that the low indicator corresponds to a low impact and that the indicator shows a relevant environmental phenomenon.

For this, the number of indicators must be limited, indicators should be determined from the data and existing models, and the calculations should be feasible in a limited time, at a reasonable cost.

Category indicators actually represent the amount of potential impact. They are distinguished by two major types, depending on their position in the causal chain between emissions and impacts: *midpoint* (intermediates) and *endpoint* indicators (final).

*Midpoint* indicators correspond to the aggregation by type of impact (acidification, destruction of the ozone layer). They are more easily accessible, with a limited uncertainty, but have a low environmental relevance. In fact, the consequences of a change in the pH of a lake or presence of a hole in the ozone layer are not accurately known (impact analysis or epidemiological study). *Endpoint* indicators correspond to the effect on targets (human health, loss of biodiversity). But they are not easily accessible, with a high uncertainty but are of great environmental relevance. In all cases, these indicators reflect transdisciplinary impacts. They must therefore be exploited by chemists, toxicologists, and cooperatively, with biologists. But it may also be very relevant to link philosophers, historians, and some epistemologists to these interpretations, especially in a perspective of survival and sustainable development of civilization. This question is all the more interesting since the choice is often complex to assume between various indicators without prioritization. Therefore, analysts tend to agglomerate indicators—in a non-factual way—to artificially help decision-making but at the expense of information that had been capitalized.

Another way of classification of impacts consists of separating them in terms of *direct* and *indirect impacts*. Direct impacts correspond to actions of sources on targets identified as the depletion of natural resources by the extraction of raw materials. Indirect impacts correspond in fact to cascades of effects: the emission and dispersion of  $SO_2$  causing acid rain, which will in turn lead to the acidification of soils, lakes, and air. The consequence of acidification will cause an alteration of the flora, the death of fish, and human toxicity, with as the ultimate consequences a loss of

biodiversity, agricultural and human productivities. The general form of an indicator is [1]:

$$Ind_i^{cat} = Coeff_i^{cat} \times pond_i^{cat} \times m_i \quad [1]$$

With:

$Ind_i^{cat}$  : Indicator of flow i for the impact category cat.

$Coeff_i^{cat}$  : Weighing coefficient of flow i in impact category cat.

$pond_i^{cat}$  : Weighing of flow i in impact category cat.

$m_i$  : mass of flow i.

Example 1:

Impact category: Climate change.

Inventory result: 20 kg of CO<sub>2</sub>, 1 kg of CH<sub>4</sub>, 0.1 kg of N<sub>2</sub>O.

Characterization model: IPCC model defining the global warming potential of greenhouse gases.

Factor of characterization: Warming potential WP.

WP CO<sub>2</sub> = 1 kg<sub>eq</sub>CO<sub>2</sub>

WP CH<sub>4</sub> = 21 kg<sub>eq</sub>CO<sub>2</sub>/kg CH<sub>4</sub>

WP N<sub>2</sub>O = 310 kg<sub>eq</sub>CO<sub>2</sub>/kg N<sub>2</sub>O

Indicator result:

Ind (WP) = (20 x 1) + (1 x 21) + (0.1 x 310) = 0.72 kg<sub>eq</sub>CO<sub>2</sub>

Example 2:

Impact category: Eutrophication.

Inventory result: 2 kg of NH<sub>3</sub>, 4 kg of NO<sub>3</sub>, 0.2 kg of PO<sub>4</sub>.

Model of characterization: Potential contribution to the formation of aquatic biomass of average composition (16 moles of N, 1 mole of P).

Characterization factor: Potential for eutrophication PE.

PE NH<sub>3</sub> = 0.35 kg<sub>eq</sub>PO<sub>4</sub>/kg<sub>eq</sub>NH<sub>3</sub>

PE NO<sub>3</sub> = 0.1 kg<sub>eq</sub>PO<sub>4</sub>/kg<sub>eq</sub>NO<sub>3</sub>

PE PO<sub>4</sub> = 1 kg<sub>eq</sub>PO<sub>4</sub>

Indicator result:

Ind (PE) = (2 x 0.35) + (4 x 0.1) + (0.2 x 1) = 1.3 kg<sub>eq</sub>PO<sub>4</sub>.



These simple examples show the complexity of the calculations of the real impacts, which depend on a significant number of inputs and outputs on the cycle of life. This is why these calculations are automatically made from databases. And from this point of view, data, reliability, update, and the accuracy of the uncertainties are at the heart of the process of life cycle assessment and of the relevance of the expected results. It can be noted that the LCA, as a decision tool, may be relevant only if reliable and accurate data are used. The confidence on some analyses must therefore always be questioned in terms of data relevancy. But when data do not exist, are not reliable and may not be retrieved, what should be decided? Should we make an LCA? Philosophical and epistemological approach could also seize this kind of thinking.

## 2.7. Interpretation of the Life Cycle

The two previous phases, inventory and assessment of the impacts, represent the area of expertise of life cycle assessment. Indeed, the approach is technical and needs numerous data. In the interpretation of life cycle assessment phase, the user, the manager, the decision maker will use the results of the impact analysis to identify the key actions that will need to be taken into account (research and development, marketing, production, financial, etc.).

The LCA results are expressed as a series of data that has both potential impacts (*example:  $X \text{ kg}_{eqCO_2}$  for the greenhouse effect*) and physical flows (*example:  $Y \text{ MJ}$  of non-renewable energy*). They are the subject of a report and, in the case of communication, a public summary document.

For an LCA comparing two products A and B, the results for each impact may be expressed for each stage of the life cycle, to compare and identify the stages presenting the greatest impacts. This can also help to compare the contribution of each product at each stage of the lifecycle. The following results (cf.

Figure 4) allow us to establish that product A presents a higher contribution to the greenhouse effect than product B for the steps of raw materials extraction and production stages, but its ability to recycle at the end of life enables it to absorb  $CO_2$ . **This representation allows chemists to identify the steps on which efforts have to be made in order to reduce impacts.**

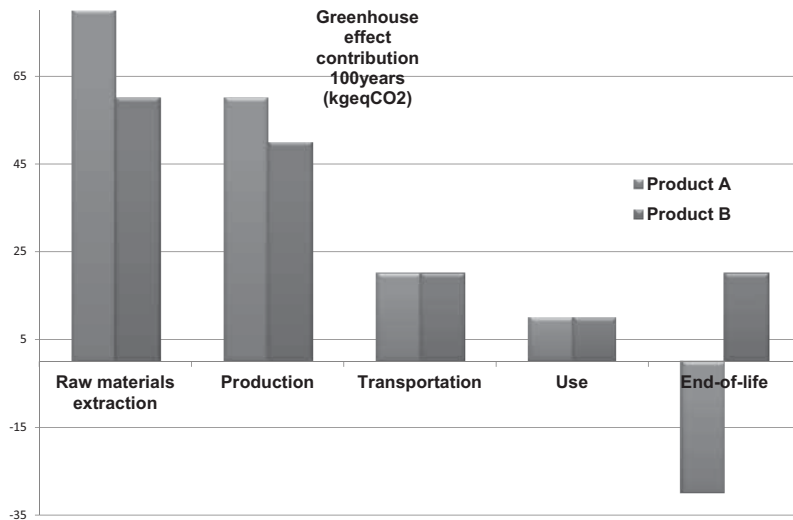


Figure 4: Contribution to the greenhouse effect of life cycle of products A and B<sup>7</sup>

Aggregation of the results for the contribution to the greenhouse effect per product allows us to identify macroscopic trends (cf.

Figure 5) but annihilates the differences in life cycle. This representation allows us to make a global selection on the product with the lowest impact.

The essential phase of interpretation is the report writing, which should contain the main elements of life cycle assessment: a reminder of the context and objectives of life cycle assessment, detailed definition of the chosen functional unit, methodology of the life cycle assessment, basic information and sources used and their limitations, encountered scientific, methodological, and technical difficulties. This report must necessarily include a critical review, i.e. the review of the study by an independent expert. This expert may act alone or within a critical review committee involving experts of the studied field and key stakeholders: **the key is to ensure the impartiality of the experts regarding the LCA in the studied domain.** Comments and responses to the recommendations resulting from the critical review should be included in the summary report.

<sup>7</sup> Author's document.

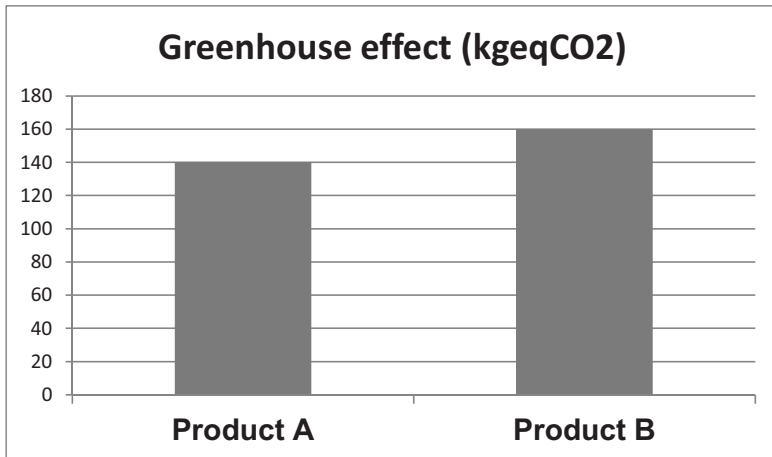


Figure 5: Aggregation of the greenhouse effect impact<sup>8</sup>

The results of an LCA can also be conveyed as an environmental statement, and are then called “Type III environmental declaration”, or “ecoprofile”, which can be printed on the product. It is the international ISO standard 14025, published in 2006, which establishes the principles and procedures for developing Type III environmental declarations and the use of the ISO 14040 series of standards for the development of Type III environmental declarations. The Type III environmental declarations described by ISO 14025 are mainly intended for inter-company communication. But their use for communication between a company and private individuals under certain conditions is not excluded. The search for improvements is the component of the life cycle assessment in which the options to reduce the environmental impacts of the system are identified and assessed. This stage includes the identification, assessment and selection of options for the improvement of the environmental load of products or processes.

Currently, life cycle assessments are most of the time used to meet certain needs such as the environmental performance of an industrial process, the environmental advertising, the comparison of environmental impacts of two products (or more), and the calculation of environmental balances.

Moreover, the initial characteristics of the product generally determine the opportunities of valorization at the end of life. Finally, this approach

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<sup>8</sup> Author’s document.

presents a strategic interest in terms of communication. Indeed, the results obtained in this type of approach may be shared with customers and provide a competitive advantage that differentiates the product from its competitors.

### 3. Innovation by Ecodesign and the Process of Integration in the Company

The LCA does not provide solutions to design products or processes of low environmental impact but is a guide to select which steps to improve. The LCA is thus a tool that helps to make choices and to guide research to promote innovation. Indeed, the results of the life cycle of a given initial product (cf. Figure 6) allow chemists to identify that the highest *impact X* is related to the production stage of raw materials. Therefore the research should be conducted on this stage in order to determine better routes or new raw materials of low impact to develop a new ecodesigned product. It is in this research process that innovation is found, and it is in this sense that eco-design is a real innovation tool.

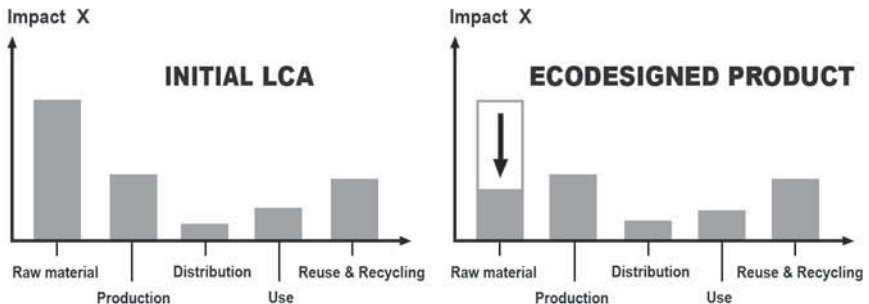


Figure 6: Innovation process<sup>9</sup>

Many examples of products can highlight the achievements of design and marketing of ecodesigned products (for example the office chair “Think” of Steelcase company- Pollutec 2004 award or the laundry Ariel cold active of P & G company). These products have been designed in the innovation process based on life cycle assessment to identify the axis of improvement related to the most important environmental impacts, the most contributing strategic steps to the life cycle. We can thus, in the light

<sup>9</sup> Author’s document.

of these examples, try to describe the integration process of ecodesign in the company in five steps and extract the appropriation process from it.

To start an ecodesign approach in a company, the first step is the *choice of the product* on which the company wants to work. This choice is made based on the product strategy studying the portfolio of available technologies, the current product range, and by carrying out a relevant benchmark. At this stage, the ecodesign approach can already point out the product and company environmental problems and enables us to estimate the environmental improvement potential of the product.

The second step defines *design goals* related to the chosen product, and will therefore have to convey the need in terms of function based on market researches and functional analysis. At this step, an initial life cycle assessment should be performed on a reference model by selecting ecodesign guidelines.

The third stage should enable one to bring out *technical solutions*, namely principle diagrams accompanied with a cost estimate. The ecodesign approach helps us to search for solutions of lower environmental impact and to carry out an environmental report.

In the fourth phase, *industrialization*, the company must optimize the production parameters, logistics, and supplies. This work is accompanied with a collection on site of impacts such as energy consumption, real mass flow, and amount of wastes, in order to conduct an environmental assessment of the final product and to prepare an environmental report.

The fifth step concerns *marketing and communication*. Distribution channels as well as possible maintenance contracts are selected. Communication about the product is carried out internally and externally based on the environmental report to establish a sales point, extract key figures, and communication media.

Beyond these five steps, this approach must also take into account the end of life of the product by providing recovery solutions for products, management, reuse, and recycling. Finally, any further development of the product (features, packaging, etc.) should be reflected on the impact assessment and communication messages.

For a company, the appropriation of such an approach lasts and involves three phases, several stakeholders and several deliverables. In a prior decision-making phase, management must confirm its involvement by the drafting of guidelines. In a first *piloting phase*, the integration process must rely on an ecodesign “pilot” experiment, with the support of management and with the help of an expert from outside the project team, from a consultancy firm that acts as a provider. After this phase, the following phase of *framing* aims at formalizing the approach in the

company, with an in-house person in charge of the coordination of ecodesign projects, helped by the outside firm to conduct internal training. In the last phase of *extension*, the approach becomes integrated to the company and is widely applicable to all design projects, coordination is carried out in-house and all members of the project are competent, in so far as the company is able to generate self-training. Management can then communicate on this approach externally.

#### 4. The Limits of the Tool

The Life Cycle Assessment is thus a particularly interesting tool because it enables a multi-criteria analysis, on the entire life cycle, without limiting itself to a single step (end of life) or a single impact (carbon footprint). In addition, this tool is standardized by the ISO standards describing it. Moreover, a same impact estimated at each stage, can be “added” to give a clear vision and helps decision-making. And finally, nothing is published without having been previously submitted to a group of experts. Thus, this tool acts as a guide to design and can be an excellent tool for ecodesign. However, if LCA can be a very powerful tool in the hands of experts, it has limitations, especially due to the complexity of its implementation. Indeed, the use of the software designed for experts and expensive databases reduces its use to a few companies and circumscribes its contribution to the analysis of products and existing methods. Its use is therefore limited to LCA experts; designers or creators are often excluded, which introduces limitations to innovation. Moreover, generally SMEs cannot afford the software, the experts, or an access to expertise level required to manage a life cycle assessment. Thus a large part of the production sector is excluded. In addition, LCA is based on the use of existing data. It is thus very risky to work on non-industrial processes with new data, which introduces limitations again.

If LCA enables the identification during a given process of the steps generating the highest environmental impacts-for example the extraction of raw materials-LCA gives a vision *a posteriori* but does not direct the course of the innovation process. In fact LCA is a study performed on an already developed or commercialized product and helps to identify the steps that have the greatest impact on the environment during the manufacture of this product. The objective of an ecodesigned process is to bring out, in a second phase, some solutions to reduce the most significant impacts during the previously identified steps. Innovation is thus born from the search for solutions during the second generation, or from the improvement of the product manufacture process. Therefore the primary

objective of these life cycle assessments is rather data compilation, the achievement of an environmental assessment, and the production of results for the communication on the manufacture of a product. The support for ecodesign is carried out a second time, because LCA is best suited to evaluate the final impact of a product rather than to guide its design. Furthermore, other limitations of this tool lie in the defining stages of hypotheses, in the allocation rules followed or the considered end of life. We will try to illustrate this through the following examples.

#### 4.1. The Importance of Hypotheses

The example of the life cycle assessment of shopping bags is very informative. This study was conducted in 2004 in France, by an expert office in LCA, for a distribution company. It was completed with a critical review organized by ADEME<sup>10</sup>. This study aimed at quantifying and comparing the environmental impacts of four types of bags available to customers in supermarkets: a single-use polyethylene (PE) bag, a reusable bag made of soft polyethylene, a single-use paper bag and a biodegradable single-use bag. The *inventory* was conducted using data collected by the bag suppliers of the distribution company and completed by the Ecobilan database.

The *functional unit* defined for this study corresponds to the service rendered by the bags: packing the purchases made by customers in stores. The *hypotheses* defined in the study report 45 visits per year per customer on average in the stores, with 200 L of purchase by visit (a cart filled to 80%), which corresponds to 9,000 L of goods per year. The functional unit was *packing 9,000 L of goods in the stores of the Group*.

The *boundaries* of the system take into account the production and transportation of materials for bags, the manufacturing and printing of bags, transport of bags, the phase of usage and the various end-of-life possibilities. The defined *inclusion threshold* is 5%. Inclusion thresholds are set at similar rates, according to usual and pragmatic practices but they can also introduce biases in the analyses: a very important toxicological impact due to an unknown impurity could alter the results.

The LCA has focused on the life cycles of the four types of bags considered. For example, the life cycle of the single-use HDPE (polyethylene high density) bag first takes into account the use and refining of oil for the synthesis of ethylene, the Ziegler-Natta catalyzed polymerization of ethylene, the production of HDPE pellets and their

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<sup>10</sup> French Environment and Energy Management Agency.

transport. These data are resulting from the inventories databases of 1999 of APME (average on 24 European sites that produce 3.87 Mt HDPE/year or 89.7% of the production of Western Europe). The life cycle also takes into account the production of titanium dioxide (data from a production site-1992), calcium carbonate (data from the Swiss Department of the Environment) and linear low density PE (average of the APME), which are the loads in the polymer. The production of glue and ink is also taken into account. In these life cycles, energy modeling is based on the energy ratios of power production of countries producing bags, namely France, Italy, Spain, and Malaysia. The differences are particularly significant for the impacts concerning the consumption of natural resources and the emission of greenhouse gases. Thus, the electricity in France is 75% of nuclear origin, whereas the electricity in Malaysia is 75% produced by the combustion of hydrocarbons. Furthermore, the calculations made to assess the impacts related to transport stages are based on the fuel consumption by trucks. The model takes into account the average consumption of a truck with full load (38 L / 100 km) weighted by one-third the mass of the load, including the influence of empty return. Finally, end-of-life stage was modeled using data from ADEME for household wastes. Thus 51% of the wastes are brought to landfills, and 49% are incinerated. And 88% of incinerated wastes are recycled to produce energy, 5% is exhausted as vapor and 22% is generated as electricity

The broad guidelines of the findings are also that the reduction of the mass of the bag and reuse of the bag are two major factors that reduce the impacts on the environment. The *conclusions* of this study are therefore very favorable to the use of soft LDPE bags—with the assumption of reuse of these bags for at least three times. But at no time is considered the possible reuse of other considered bags (including HDPE and biodegradable bags, which could be reused a second time, or at least as garbage bags). In addition, the study compares bags with very different volumes, which involves quite variable amounts of material depending on the bags. And yet knowing that the mass of the bag is an important parameter, it would have been appropriate to consider the solutions showing larger volumes for the same bag. Thus, we can clearly identify that the LCA evaluates selected products and helps in choosing the best product *within this* selection. However experience shows that solutions to a problem can often be located outside a pre-selection. ‘The relevance of a problem sometimes resides outside the data used as input. We must imagine the reality outside the available data to apprehend it. In this respect, we must imagine what is not known. Pose or model a problem, it



is often to distort it and open towards false solutions'. We must be innovative to really find ecodesigned solutions.

The example from the study of Kim and al is also very illustrative of the importance of choosing the hypotheses of the LCA. Indeed, in their study, this team compares the environmental impacts of two types of polymers, polystyrene PS—obtained from polymerization of styrene, a monomer coming from oil, and a polyhydroxyalkanoate PHA—polyester derived from the fermentation of sugars extracted from corn kernels, from agricultural origin. The comparison is carried out at identical mass, despite any possible differences in properties. The results presented in this study show firstly that the impact on the greenhouse effect is lower in the case of the manufacture of polystyrene (2.9 kg<sub>eqCO2</sub> for the PS and from 3.5 to 4.4 kg<sub>eqCO2</sub> for PHA). However, secondly, the production of sugar from by-produced straw and also the recovery of energy derived from the valorization of straw are added in life cycle. And in this second case, the production of PHA becomes a CO<sub>2</sub> well, to the extent that the indicator is -1.2 to -1.9 kg<sub>eqCO2</sub>. This example perfectly illustrates the importance of choosing the right hypotheses and limits on the final result.

## 4.2. The Relevance of Inventory Data

Concerning the life cycle assessment of bags described in part 4.1, the LCA has studied the *life cycles* of four types of bags. For example, the life cycle of the single-use HDPE bag first takes into account the exploitation and refining of oil for synthesis of ethylene, the Ziegler-Natta catalyzed polymerization of ethylene, the production of HDPE pellets, and transport. However, these data come from the inventory databases of 1999 APME (average on 24 European sites that produce 3.87 Mt LDPE/year or 89.7% of the production of Western Europe). And yet in the study we learn that the HDPE is manufactured not only in France, but also in Asia and Brazil. Not only do the inventory data from APME related to the manufacture of HDPE date back to 5 years, but also they are not representative of manufacturing in Brazil or Asia—they cannot be used to assess the environmental impacts. Similarly, the life cycle of the HDPE bag also takes into account the production of HDPE bags. In this case, the data come from inventory databases of APME (average on 8 sites for the production of the United Kingdom 1993). And yet these HDPE bags are manufactured in France. Thus not only are these data old (more than 10 years) but they also represent only part of the British situation and can never be representative of the French situation—in terms of energy consumption only. Indeed, if the electricity production in France is mainly

nuclear (78%), then thermal (11%) and renewable (11%), this ratio is completely different in the United Kingdom where electricity is mainly of thermal origin (75%), then nuclear (20%) and renewable (5%). Thus, environmental impacts are completely different (contribution to global warming) and cannot be used from one country to another.

### 4.3. The Influence of the Allocation Rules

The rules for allocating wastes can also play a crucial role in the results a life cycle assessment. Thus, if we compare two LCA on bioethanol as biofuel (an LCA conducted by ADEME in 2002 and another one conducted by EDEN in 2006), the results are very different. Indeed, the energy performance of bioethanol of wheat (returned energy / mobilized renewable energy) varies from single to double for both studies: 1.10 for EDEN; 2.05 for ADEME. These differences may be explained by the differences in the choices made for the allocations of waste from bioethanol. Thus, EDEN has chosen to include in its LCA all of the impacts generated by the wastes from the bioethanol sector, thereby promoting a systemic approach, while ADEME allocates only 43% of the impacts of waste to bioethanol. ADEME has made the choice of mass allocation for its LCA –bioethanol, product targeted by the sector, representing only 43% of the mobilized dry matter. These two options can be selected but it is important to understand that the results can be radically changed.

### 4.4. The Choice of Recycling

Concerning the end-of-life, the comparison of different paths of valorization is crucial. Indeed, it is usually impossible to directly compare the environmental impacts generated by two ways of valorization of a product. If we wish to process 1 ton of waste paper, we cannot directly compare *recycling*-that will produce  $Y$  kg ( $Y < 1000$ ) of recycled paper-and *thermal valorization*-that will produce a quantity  $X$  MJ of electricity. Indeed, in the first case, we will always need a power production and in the second case, we will still need paper-these two systems do not render the same service. It is therefore necessary to complete this comparison by adding to each system the process avoided depending on the chosen option (cf. Figure 7).

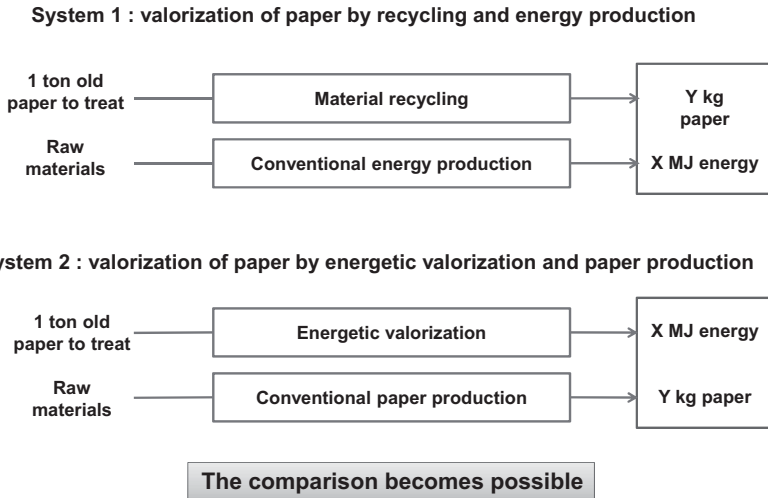


Figure 7: Comparison of both completed systems<sup>11</sup>

Thus, in the first case (paper recycling), we must also take into account in the impact assessment the production of X MJ of electricity depending on local conditions of conventional electricity. And in the second case (the thermal valorization), we must also consider the conventional production of Y kg of paper from wood in the impact assessment. We can now compare strictly two systems that have the same products: Y kg of paper and X MJ of electricity.

The LCA is therefore an interesting tool because it enables a multi-criteria analysis, on the entire life cycle, without limitations to a single step (end of life) or a single impact (carbon footprint). This tool is standardized through the ISO standards that describe it and guarantee an expert review before publication. And a same impact estimated at each stage can be “added” to give a clear vision and help decision-making. However, this tool has some limitations that particularly lie in the rigorous selection of the hypotheses definition, limits, and functional unit. Similarly, the followed allocations rules or the considered end of life may significantly change the results. But the more restrictive limitations of this tool are methodological and qualitative. Indeed, the calculated impacts are potential impacts and do not reflect the local reality. In addition, this tool is not dynamic. Thus, data inventories, even when they come from

<sup>11</sup> Author's document.

measurements on site, are valid for a limited time and are scarcely updated. And the quality of the data may be questionable. When the data are derived from databases (European average or other), they are not necessarily representative of local realities and are also limited by a low frequency of updating. In all cases, the results are only rarely updated. More importantly, LCA does not take into account the margin of technological progress that it compares. In fact if we compare a very well established and highly optimized technology with a new technology, it may be necessary to conclude that the first older technology causes less environmental impacts without realizing that the new technology has more room for progress. And we can thus decide not to develop this new technology even though it would cause less impact after a few optimizations. LCA eases everything and does not include time as dimensional variable.

## **Conclusion: The Future of Ecodesign**

Design processes in industry and in particular in chemical industries are now changing. They must respond to a holistic challenge of reduction of environmental impacts at each stage of the manufacturing process. They must integrate ecodesign of the product or process. In this approach, life cycle assessment LCA is a crucial tool for environmental assessment. And, in doing so, life cycle assessment, by identifying the progress margins in terms of environmental impacts, energy and resources consumption, becomes a strategic tool for innovation. This tool enables us to guide Research efforts and development, thereby leading to the identification of innovative solutions to reduce environmental impacts, to lead to new products, which are “greener”, ecodesigned, and responding to the more and more pressing demands of the market and regulation. However, the process of life cycle assessment is carried out *a posteriori* on an existing product or process and helps us to analyze the environmental impacts of this product or process. The results of this LCA thus highlight the steps that have the greatest impact on the environment. We will have to work on these steps to reduce the environmental impact, but only during a phase of product improvement or during the design phase of the “second generation” of this product. In the first approach, life cycle assessment enables us to compare the environmental impact of two products to find the best compromise. However, we have seen previously that the solution of a problem may lie outside the selected elements, as the ecodesigned solution. Therefore, this LCA tool has to evolve to make it more usable in an innovation process. But the more restrictive limitations of this tool are

methodological and qualitative. Qualitative because the relevance of the data is essential when assessing impacts and because these data are not always relevant or updated in the databases, they are not always representative of local reality. Methodological as this tool enables a comparison in time, an assessment of the relative impacts and does not take into account the margin of technological progress that it compares. Moreover, the definition of the hypotheses, limits, the functional unit, and the followed allocations rules or the proposed end of life, can significantly alter the results. Thus, it is highly desirable that this life cycle assessment tool evolves, remedies these limitations, and better assesses impacts related with toxicity and nuisances.

In addition, to meet the new constraints in the innovation process, to be upstream of the project phases, to support the design of the products and processes in the chemical industry, and to take into account the new regulatory aspects, new tools are needed, which will provide guidelines to be followed to guide the choices of researchers and chemists. It becomes more and more important to assist the innovation process with a tool that helps piloting, “*gate to gate*”, instead of concluding it from a comprehensive analysis *a posteriori*. And it is important to extend this environmental design to all projects in the chemical industry to make ecodesign emerge in this industry. To do this, designers of products and processes in the chemical industry need a suitable tool, easy to use and not just made for environmental assessments experts, a tool that can guide them from the choice of access route on final environmental impact. Industry must also extend the collection of inventory data and share these inventory data to contribute to update the inventory databases, which is a real “Achilles heel” of LCA. Moreover, it is crucial to link inventory databases to those classifying dangerous substances. How can we imagine nowadays the identification of a chemical access route without anticipating the constraints imposed by the regulation and in particular the REACH regulation? It is also crucial to be able to generalize the use of such a tool to smaller companies to increase their competitiveness. It is thus necessary to provide them with a tool usable at all stages of the project, early in the phases of innovation, including guiding the choice of R & D. Existing tools do not necessarily respond to this objective, particularly for SMEs in the chemical industry, which are looking for a simplified reference frame to enable them to integrate the concept of sustainable development in the design of their products. Thus, if quality management started in 1992 for major groups, these actions have only started around 2004-2006 for smaller structures. Nowadays, in the industrial sector, only a quarter of companies provided for the end of life

of their product, and there are ecodesign practices among 40% of them. Finally, it is essential for companies to take over the involvement in Research and Education and to help to mobilize the Academic Research teams in this area.

In all cases, the eco-design is a crucial concept, generating changes in chemistry. Indeed, it requires adopting a holistic analysis of the processes and holistic approach. It enables us also to justify the choice of low environmental impact pathway or to avoid a path that only seemed better *a priori*: it is a decision-making tool that helps to reduce environmental impacts. Therefore, if chemists, engineers, biologists, toxicologists, and ecotoxicologists are involved, it seems very important to involve historians, philosophers, and epistemologists in the interpretation of the results of LCA in a dynamic of sustainable development of civilization. Indeed, the notions of negative externalities-environmental impacts-must be considered in the light of the progress made in a historical and philosophical perspective. As life-cycle assessment is only an environmental analysis and since a societal analysis should be added-through societal life cycle assessment-the place of historians, economists, and philosophers may be further increased. Finally, ecodesign induces an evolution of all processes proving the interest of reuse, recycling, and circular economy. Indeed, the increase of life duration, the extra life cycles, is the preferred axis of reduction of impacts. As the maxim of Antoine de Lavoisier, stating in substance the first principle of thermodynamics ‘nothing is lost, nothing is created, everything is transformed’, ecodesign aims to reduce losses and new creations and promotes the (re)transformations. And this circular evolution of the economy and chemistry resources (initially renewable resources, and then coal and oil, and from now more and more renewable) must also be supported by the thinking of historians and philosophers.

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# THE PRECAUTIONARY PRINCIPLE AND CHEMICAL RISKS

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## Introduction

The precautionary principle (PP) is a relatively new anticipatory model that public authorities may legitimately apply—or in fact *should* apply—when faced with scientific uncertainty about possible harm resulting from human activities in relation to environmental protection, public health or food safety. Over the last twenty-five years it has developed as a policy and as a legal concept, mainly in Europe. A key date in the foundation of the principle is firstly in 1992, when it was mentioned in the Maastricht Treaty as one of the basic principles governing the European Union’s environmental policy; and secondly, through its incorporation into Principle 15 of the Rio Declaration adopted in June that year by the Rio Summit, it received acknowledgement in the international arena, albeit in a watered-down format deprived of legal strength, known as the “precautionary approach”.

Both the principle and the approach are relevant to address collective “potential risks” or “hypothetical hazards or threats”. These expressions refer both to hazards, the existence of which is scientifically uncertain, being neither proven nor refuted, and to dangers for which, despite their known existence, there is no realistic way to establish credible probabilities for the damage scenarios they may entail<sup>1</sup>. The adjective “collective” means that individual agents are not in a position to control these risks (see Box 1) or hazards singlehandedly, although they may have some ability to protect themselves against them. Influenza provides a typical example of where collective risks are ascertained to affect public health. As such, environmental risks are “collective” in essence: think of

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<sup>1</sup> For those who are concerned by the objective foundation of probabilities, the latter can only be reached either by logical or theoretical analysis, or by statistical observation of repeated events belonging to the same class.

dangerous alteration of the global climate or the depletion of stratospheric ozone.

By contrast, “prevention” usually addresses known risks for which a full risk assessment can be delivered, leading to quantitative estimates of the exposure of various groups and of the expected damage. As such, prevention is highly demanding in terms of knowledge and information but, since it is based on reasonably precise estimates, it offers a rational basis for policies, for the ability of social security institutions to cover the risks by anticipating the costs, and for the business of insurance companies. Scientific uncertainty, on the other hand, does not lend itself so easily to precautionary action. For this reason, prior to the mid-1980s, hazards, dangers and threats that were difficult to define were subject to on-going research whilst being disregarded by safety policies. At the same time, scientific uncertainty is not a simple issue for the insurance industry to address, and an increase in exclusion by insurance companies during the last few decades has reinforced the interest in precautionary measures for limiting the likelihood of damage.

***Box 1: difficulties with the word “risk”***

The word “risk” means different things to different people. It has a certain meaning for insurance companies, such as flood risks or car accident risks. If risk is defined as “a function of the probability of an adverse health effect and the severity of that effect, consequential to a hazard”, as in article 3 of the EU regulation 78/2002 on food law and food safety (European Council, 2002), then this is not consistent with the expression “potential risks”, since it describes situations for which it is not possible to state an objectively and scientifically established probability. If risk is defined by the stochastic nature of the consequences of an action, with the stochastic range being expressed around a central value, the term “potential risks” is also inappropriate, since it relates exclusively to the possibility of harm attributable to the exposure to danger. In fact, common usage and public debate have given a meaning to the word risk that is different from its neutral meaning in decision theory. Its everyday meaning is “danger”, “possible damage” or the “threat of disaster” with no explicit consideration of probabilities. In this paper I use the word risk in its most extensive meaning, to encompass situations that decision theory would term as risks and also those it would consider as uncertainty.

In spite of a general agreement that scientific uncertainty delineates the PP's field of relevance, very different competing interpretations of what the principle requires as a policy norm have coexisted from the very beginnings and still do today. Yet by the year 2000 the European Union and member states had developed a doctrine that fixed the terms of what the PP meant for them and what, in their understanding, it did not. In spite of this, there is no other policy concept that continues to raise as many misconceptions and misunderstandings as the PP: many feel that they have a legitimate right to define the PP according to their own terms, scrutinizing public management and condemning government failure to implement his or her own preferred PP. In spite of this divergence, most people refer to the PP, as if it was a unique and commonly understood concept. In this regard the biggest contrast can be found between the EU's PP and a catastrophist approach to uncertain hazards. At the same time the logic of compromise at work behind EU statements and rules has sometimes resulted in EU governance texts that contain ambiguous wording or contradictory uses of concepts in relation to the implementation of the PP. This is shown in the context of the REACH regulation that addresses chemical hazards.

The first objective of this chapter is to introduce the fundamental doctrine of the PP that was adopted by EU institutions (Commission, Council and Parliament) in 2000; the EU being the only large region where something called the PP has been implemented and controlled by case law. The second aim is to underline the contrast between this doctrine and other views that have been put forward by stakeholders from non-governmental organizations (NGOs), close research partners, and a few other academic people. I then address chemical products, beginning with a question on the specifics of chemistry in relation to science and risks. Finally I consider the REACH regulation and reflect on the extent to which it may be seen as a sensible implementation of the PP.

## **1. Discrepancies between the PP as a Policy Norm, A Concept of Rational Decision Theory, and A Negotiated Political Tool**

In the literature there is no agreement on what the specifics of the PP really are. On one side, NGOs and their academic counterparts take firm positions on the PP as the main force to trigger a desired divergence with existing risk management and technological development modes, but at the price of the advancement of often inconsistent or unreasonable requirements, as will be further explored below. While on the other side,

authors grounded in decision theory confront great difficulties in order to grasp what it is that the PP really brings as a social and legal norm. Then, there are several discrepancy types to be considered that can be classified in relation to the following poles: first there is public doctrine, adopted in legal texts and political statements, echoing institutional cultures shaped by history; second there is what activist NGOs ask for regarding risk management; third there is what governments actually do and fourth, there is the academic debate on the PP oriented by researches on rational behaviour under uncertainty (See Figure 1).

Figure 1: Mapping the discrepancies raised by the Precautionary principle.

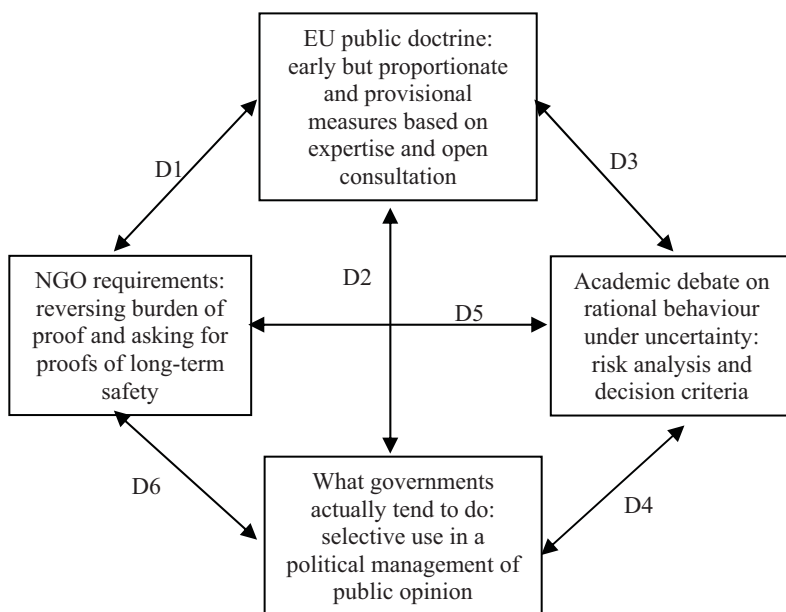


Figure 1 shows how discrepancies are spread between the four identified poles. In order of importance, the most significant type are D1 (conflicts between the public doctrine and NGO requirements); D2 (between the public doctrine and real-life public policies under pressure or lack of it from social movements and public opinion); D3 (those between the academic framing of concepts and the EU's public doctrine); D5 (between academic recommendations on rational management and the requirements of NGOs); and D4 (between academic framing and real-life management by governments). It is clear that the discrepancies differ

according to the issues involved, such as: GMOs, agricultural chemicals, BSE, climate change, nanotechnologies, etc.

Let us consider a D3 example. In his recent reviews, Charles Vlek (2010a and b) places the examination of the PP in the context of a search for a basic rational attitude for complex, ill-defined, uncertain and potentially catastrophic situations. He does not see substantive differences in problems for collective decision-making and for individuals in their everyday lives (financial investment, medical treatment, road transport and extreme sports); nor does he consider that specific fields of concern warrant special attention, such as environmental and public health protection versus profit-making financial investment. The author regards the PP as relevant for every practical domain of action and discusses it as a general standard for rational decision-making, not as an original policy norm that is valuable for certain fields.

This framing is problematic. The dominant Bayesian theoretic framework does not make conceptual distinctions between risk and uncertainty. According to Savage's argument (1972) all probabilities are subjective since they imply a level of confidence in information provided by others (scientists, experts) or directly obtained through experience. In this way, any uncertain situation can be supposedly understood within a subjective probabilistic framework. At the same time, it is the objective of decision-theorists to deliver relevant policy-making analyses that touch on uncertain risks, as if policy-making were just an exercise of applied decision theory. Thus, from the academic viewpoint, the PP has difficulty escaping from being considered as either highly disputable or intrinsically flawed, whenever it calls for extreme obligations of abstention in response to any potential risk (Sunstein, 2005), or re-joins standard criteria developed in probabilistic Bayesian theory. At best the PP is given a psychological foundation in the particular attitudes of extremely prudent agents<sup>2</sup> for whom the prospect of gaining better knowledge<sup>3</sup> in the future paradoxically induces an increase in resources allocated to immediate precautionary measures, compared with a situation of no improvement of knowledge (Gollier, Jullien, Treich, 2000).

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<sup>2</sup> Formally the absolute prudence index should be at least twice as high as the index of absolute risk aversion ( $P \geq 2A$ ), knowing that the prudence index is assumed to be expressed by the ratio of the third derivative to the second derivative of the von Neumann-Morgenstern utility function. Note that these derivatives are not observable.

<sup>3</sup> This is the way these authors interpret scientific uncertainty: as the promise of better knowledge tomorrow than today; and the prospect of better knowledge is supposed to increase the uncertainty perceived *ex ante* by very prudent people.

At the intersection of academic literature and more policy-oriented reflection, Vlek (2010a, p. 533) identifies three distinctive features of the PP: the inclination to take a pessimistic view of possible outcomes; the proponent's burden of proof to demonstrate that new actions are likely to be safe; and a tendency to delay risk-taking until sufficient new information becomes available. He concludes, "the basic motive for being precautionous lies in the asymmetric presence of possible serious harm or damage vis-à-vis moderate expected benefits" (ibid, p. 535).

He then compares the PP to the Venture principle (VP), the latter involving uncertain highly attractive benefits with moderate risks of loss. The discussion is interesting, but does not wholly grasp what the PP really is in terms of the EU's public doctrine. The three features identified by Vlek are not in fact constitutive of the EU's PP doctrine, which does not insist upon either a systematic premium being given to the consideration of potentially bad outcomes, or to a reversal of the burden of proof, but the central idea of which is to take account of hypothetical risks early on in the process, which should not be confused with the systematic delay of risk-taking.

This illustration provides an example of a more general observation: unfortunately, a large part of academic decision-theoretical literature that sets out to define and discuss the PP either misses the target or overemphasizes the peripheral aspects of the PP. This is not to say that such literature has an absolute lack of relevance, since many present very good arguments against certain usages of the PP by authorities, or against certain demands from industry or NGOs.

The PP brings innovation to risk management, but its novelty does not lie in the fact that the PP would systematically express a more precautionary attitude, in the ordinary sense, compared to previous prevention policies, for instance by increasing safety margins, focusing on worst-case scenarios, or by allowing a strong aversion to risk to dominate decision-making. The practical novelty of the PP is to put insufficiently known and uncertain hazards from the field of environmental protection and public health into the domain of public attention and action, especially in situations where there are threats of huge and irreversible damage.

It first implies a social value choice, considering that environmental protection and human health take precedence over economic profitability when conflicts arise. Secondly it rehabilitates the old distinction between uncertainty and risk (Knight, 1921; Keynes, 1921), i.e. between hypothetical hazards that are surrounded in uncertainty and are not amenable to probabilistic calculations, and recognised risks that do facilitate probabilistic calculations and fit the standard concept of prevention. In

essence, the Bayesian and Savage approaches to risk are not capable of making this distinction between prevention and precaution.<sup>4</sup>

These foundations having been laid, the foremost component of the PP is that it demands an early account of possible hazards in spite of scientific uncertainty: authorities should not wait for full scientific certainty and should not use uncertainty as a pretext to postpone measures that address possible hazards. Thus the main innovation provided by the PP is that it changes the time schedule of the creation of policies in relation to risks, in favour of providing an initial account of uncertain risks (Godard, 1997; European Environmental Agency, 2001). At the same time, informed ignorance, i.e. ignorance that remains after having mobilised existing sources of scientific information, along with the simple assumption that “bad effects could happen” are not sufficient to mobilize the PP. It is the cognitive grey areas that exist between ignorance about the possible risks and the well-known risks that constitute the focus for the principle.

## **2. The Conceptual Context**

### **2.1. Scientific Uncertainty**

Scientific uncertainty delineates the background to the PP. Ascertaining what scientific uncertainty actually is raises difficulties for risk managers. It should not be confused either with the when and where uncertainty of contingent events that occur in every life, such as “when will the next flood occur in New Orleans?”, or with general ignorance. Scientific uncertainty should also not be confused with a complete lack of information about the possible outcomes resulting from the use of a technology, but should be seen as a lack of conclusive scientific knowledge about the laws, processes, mechanisms or properties of specific natural phenomena, such as changes in the behaviours of substances when organized at the nanoscale, or detrimental processes induced by non-conventional pathogens. Scientific uncertainty does not refer to the state of knowing nothing, but to when one’s knowledge is inconclusive and remains at the stage of unresolved hypotheses and conjectures, although derived in accordance with standard scientific approaches and empirical observations.

With this background, scientific uncertainty may affect risky situations at different points. We may have uncertainty in the realization of harm:

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<sup>4</sup> Economic approaches developed within a Bayesian framework are presented in Kast and Lapied (2004) and Gollier (2004).

harm may just be a possibility that has been neither dismissed nor proven. There may also be uncertainty in the causes of a given phenomenon: for example, while damage to health or a detrimental process affecting the environment may have been observed, the causes may remain unknown. Both types of uncertainty are derived from insufficient knowledge on the relationship between active causes (a technology, a substance) and detrimental effects.

Scientific uncertainty constitutes a challenge not only for experts and managers, but also for the legitimacy of public action: welfare states and public action in Europe have been developed on the basis of a rational-legal model for which establishing objectivity of issues is a critical feature for enabling decision-makers to act in accordance with the general interest and to obtain confidence and support from public opinion. When faced with uncertainty, individual agents may shape beliefs about the probabilities of ill-defined events, such as catastrophes, based on a mixture of piecemeal information and personal attitudes and values. This may lead to the formation of subjective opinions regarding the riskiness of situations. These psychological constructs are nonetheless deprived of direct relevance as a basis for reasonable public action, except when setting ultimate political limits of social acceptability under a democratic regime in contexts marked by high stakes and strong social controversies.

Indeed policy-making in democracies entails another requirement, that of justifying goals and actions to citizens with the help of analyses and arguments that can be shared with a majority of citizens. A symmetrical obligation to ascertain positions and proposals is addressed to citizens that make various demands. So, both governments and citizens have to justify the actions and policies they propose, whereas respective arguments are open to discussion. In this context, scientific expertise aims to reach shared statements that approach objectivity and enlighten decision-making. At stake is the definition of a common world on the basis of which public deliberation may take a reasonable form despite unavoidable trade-offs between interests and concerns.

Scientific uncertainty jeopardizes the possibility that citizens can share an objectively determined common world, making public deliberation difficult, controversial and inconclusive, unless there is agreement throughout society on how to address hypothetical risks. This critical link between public decision-making and objectivity explains the huge role of scientific expertise in public decision-making in relation to risks to the environment and health. Unfortunately the search for an objectively determined common world is generally ignored by academic work from the decision theory field due to its individualistic and subjective approach.



For the advocates of the latter, problems of public decision-making are only linked to procedures for aggregating the individual preferences of consumers, or to how public decision-makers can manage various sources of information and influences in order to maximize their own utility function (power, career, wealth, honours).

Since scientific uncertainty does not allow objective probabilistic formulations, supplementary points of support must be found to make reasonable decisions: this requirement provides the legitimacy for more extended procedures of public debate and dialogue with interested parties in parallel to scientific expertise and normative assessments produced by lawyers, economists and ethicists. With this three-way approach, the PP clearly calls for case-by-case consideration to elicit judgments on proportionate and provisional measures to target potential dangers or uncertain threats.

## 2.2. The PP as a Principle

Principles are different from rules and criteria (Godard, 2010): various principles may coexist in spite of contradictory implications; they do not establish a complete order on a set of actions; they are compatible with different—but not all—criteria.<sup>5</sup> For instance in spite of what is often said (Gardiner, 2006), the PP is not to be identified with a maximin criterion. So the question is raised: why are principles useful? Their purpose is to provide a broad base for more precise rules and criteria valuable for particular circumstances; in doing so, they link agreed social values and legitimate forms of commitment to action in rather abstract terms. They establish a meaning that gives direction and clarifies existing or proposed institutional procedures. They are a reference point in a coordination process that must accommodate numerous transformations and wide empirical diversity. Ultimately, they stimulate change in an existing normative system (de Sadeleer, 2003). Many criticisms addressed at the PP—that it is vague, unclear and inoperable—in fact fault it for being a principle, and not a criterion, which is just nonsense.

## 2.3. A Conceptual Heritage

The explicit formulation of the PP goes back to the German *Vorsorgeprinzip* in the 1970s. It then combined two main ideas: a) not

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<sup>5</sup> See Vlek (2010b) for a review of possible decision-making criteria to be used for the implementation of the PP.

waiting for the stage of scientific certainty on causal relationships involved before undertaking preventive action designed to limit or avoid environmental threats; and b) committing to a long-term, continuous and adaptive approach to environmental measures, by being opportunistic in the use of technological progress to drive ecological modernization of industrial processes.

These two ideas were somewhat separated by the events that followed: the second became part of the concept of sustainable development, while the first emerged as the PP. Meanwhile both remain compatible and even complementary. As the 2000 Nice Resolution on the PP (see below) stated, the PP must be understood in the light of sustainable development.

In France the 1995 law 95-101 for the strengthening of environmental protection defined the PP in the following terms: "Absence of certainty, taking account of current scientific and technical knowledge, should not lead to the postponement of the adoption of effective and proportionate measures aimed at averting the risk of serious and irreversible damage to the environment, at an economically acceptable cost."

In May 1998, the European Court of Justice issued a judgment on the mad cow disease case between the UK government and the Commission; it then confirmed the PP in substance by reckoning that the authorities were justified in taking health measures without waiting to have full scientific certainty about causal links and the extent of damage. For the first time this decision gave the PP an autonomous legal force in an area other than that of the environment: food and health safety (European Court of Justice, 1998; Gonzalez Vaqué *et al.*, 1999).

Following a request from the European Council and an open consultation process with stakeholders, the Commission released a communication on the PP in February 2000. This key text expounded the doctrine that would inspire the Commission's policy in the field of environmental risks (European Commission, 2000). It places the PP in the context of risk analysis according to agreed international standards, in spite of the fact that risk assessment cannot be conclusive. Concepts of proportionality, coherence and regular revision of measures are stressed, as well as the need for public authorities to organize an independent, competent, multi-disciplinary, transparent and adversarial expertise. On this basis, a "Resolution on the precautionary principle" was adopted by European heads of state and governments at the Nice summit in December 2000 (European Council, 2000), which was soon followed by a symmetrical statement from the EU Parliament. These convergent documents gave political legitimacy to a specific, "proportionate" doctrine

of the PP, which confirmed the main ideas already present in the Rio Statement and the French law.

In 2002, the European regulation 178/2002 on food safety was adopted. It poses a principle in Article 14:

Food shall not be placed on the market if it is unsafe. Food shall be deemed to be unsafe if it is considered to be (a) injurious to health; (b) unfit for human consumption.

This requirement for safety should be assessed by taking the normal conditions of use and information given to consumers into account. It also made the PP one of the pillars of food safety regulation. Article 7 under the title “Precautionary principle” states:

1. In specific circumstances where, following an assessment of available information, the possibility of harmful effects on health is identified but scientific uncertainty persists, provisional risk management measures necessary to ensure the high level of health protection chosen in the Community may be adopted, pending further scientific information for a more comprehensive risk assessment.

2. Measures adopted on the basis of paragraph 1 shall be proportionate and no more restrictive of trade than is required to achieve the high level of health protection chosen in the Community, regard being had to technical and economic feasibility and other factors regarded as legitimate in the matter under consideration. The measures shall be reviewed within a reasonable period of time, depending on the nature of the risk to life or health identified and the type of scientific information needed to clarify the scientific uncertainty and to conduct a more comprehensive risk assessment.

From this, specific actions and informational obligations for the agri-food industry have been established: whenever an operator suspects the safety of food ingredients that have been bought, processed or occur in food products that have been put onto the market, there is an obligation to withdraw these products and to inform the relevant authorities, and also the affected consumers if the products have already reached them (European Council, 2002). On intellectual grounds, this regulation had already suffered from the inner tension that REACH would know a few years later and that occurs between the requirement for safety and the state of scientific uncertainty. What is safety in uncertain contexts? How can safety be ascertained in situations of scientific uncertainty?

In March 2005, the French Congress added an Environmental Charter to the French Constitution, giving a constitutional value to the goal of environmental protection and stating that public policies must aim at

sustainable development. It refers in Article 5 to the obligations of the public authorities in implementing the PP:

If the occurrence of damage has the potential to affect the environment in a serious and irreversible manner, even though there may be scientific uncertainty, the public authorities should make sure, by applying the precautionary principle and within the limits of their attributions, that risk assessment procedures are followed and that provisional and proportionate measures are taken in order to preclude the occurrence of damage.<sup>6</sup>

This article emphasizes the imperative responsibility that public authorities have in organizing the implementation of the PP, as well as for implementing appropriate risk evaluations and for taking appropriate measures that are both proportionate and provisional.

Following a Chemicals White Paper issued by the EU Commission in 2001 (Rogers, 2003), the REACH regulation entered into force in spring 2007. This regulation targets chemical substances not already covered by existing regulations. As indicated by the REACH acronym, this regulation introduced new obligations and procedures aiming at registering, evaluating and authorizing—or forbidding—tens of thousands of chemical substances, both existing and new. Special attention is given to chemicals classified as carcinogenic, mutagenic or reprotoxic (CMR), or as persistent organic pollutants (POP). Whereas previously chemicals could only be banned if proven to be dangerous, REACH requires EU industry and importers to prove that each substance intended for the market is safe for human health and the environment. This is what is sometimes referred to as a reversal of the burden of proof. However, “reversal” is an excessively strong word as this idea is in fact impossible to satisfy, given that it is not possible to prove the absence of future damage as science is always incomplete and on-going; proof is limited to existing tests and established knowledge and there is no possibility of dismissing future scientific progress and discoveries on new types of harm. Here the inherent contradiction in the wording of REACH is revealed, which can only be overcome by adding subtle conditions and provisions in the evaluation-authorization process.

### **3. The Precautionary Principle in the EU Doctrine**

Two main texts express the PP doctrine of the EU: the Communication presented by the Commission in February 2000 and the Resolution adopted by European heads of state at the Nice Summit in December

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<sup>6</sup> Unofficial translation from the French.

2000. These texts have no direct legal force, but delineate a politically legitimate conception that should inspire action by the Commission and across all member states. It should also stimulate legal decisions by jurisdictions and in particular the European Court of Justice.<sup>7</sup> This doctrine is summarized in Box 2 (below).<sup>8</sup>

**Box 2: The EU doctrine on the precautionary principle**

1. *The PP is to be applied if the scientific information is inconclusive and there are reasonable grounds for the concern that potentially dangerous effects on the environment, human, animal or plant health may be inconsistent with the chosen level of protection. The possibility of harmful effects on health or the environment has to be identified through scientifically recognized procedures where the preliminary scientific assessment of available facts and scientific results does not enable the determination of the risk with sufficient certainty.*
2. *The PP is to be understood and implemented within a sustainable development perspective.*
3. *To proceed to an assessment of the risks, the public authority should have an appropriate research framework, drawing in particular on scientific committees and relevant scientific work; public authorities are responsible for organizing risk assessment, which should be conducted independently and transparently on a multidisciplinary basis; open debate and adversarial procedures should be enhanced. The assessment of the risk should allow the mention of minority views in public reports.*
4. *Civil society should be implicated and particular attention should be paid to consulting all interested parties at the earliest possible stage.*
5. *The whole spectrum of measures able to achieve the desired protection level should be considered, including the no-action option. The choice of measures should respect the principle of proportionality by taking into account short and long-term risks and by aiming at the high level of protection sought; the least restrictive measures for trade should be sought under the condition that they reach the desired level of protection. Measures should be consistent with those already taken in similar situations, taking account of the most recent scientific developments and the evolving level of protection sought.*
6. *Measures taken on the basis of the PP should be re-examined in the light of the development of scientific knowledge. To this end, follow-up of the effects of decisions should be implemented and further research carried out to reduce the level of uncertainty.*

<sup>7</sup> In this regard, see Stokes (2008) and Rogers (2011).

<sup>8</sup> See also Klinke *et al.*, (2006).

As synthesised by Rogers (2011), the EU PP adopts five components for screening precautionary actions:

- Proportionality to the chosen level of protection.
- Non-discrimination, in particular in regard to imported products.
- Consistency with similar measures previously taken for known risks, but taking account of scientific progress and the changing concerns of society.
- Choice of measures based on the consideration of the potential benefits and costs or various possible actions, including the no-action option.
- Periodic review of measures in the light of new scientific results.

### **3.1. Application Field and First Order Responsibility**

The relevant field for the legal application of the PP is limited to the environment, the health of animals and plants, human health, food and feed. The PP applies both to the Commission's policies and actions and to those of the member states. Public authorities stand at the forefront of the organisation of appropriate PP implementation: they are responsible for setting-up scientific assessments and launching dedicated research actions in order to elucidate unresolved scientific uncertainty. They bear the political responsibility of estimating the right level of acceptable risk, though they should remain in line with the EU objective of ensuring high levels of protection for health and the environment, with principles of proportionality and consistency regarding the measures adopted in similar situations, and with international trade law, particularly concerning the Agreements on Sanitary and Phytosanitary measures (SPS) and the Technical Barriers to Trade (TBT) (Belvèze, 2003).

### **3.2. Proportionality**

Proportionality is an important ingredient of the EU doctrine. This word is a clear affirmation that the PP does not embrace catastrophism (see later) as the relevant framing to address hypothetical risks. The PP plays a role in a type of risk management that aims for a high level of environmental and health safety, but its purpose is not to condemn all risks or to guarantee that no damage could ever occur. Moreover, the objective is not to minimize possible damage at any cost. In other words, the PP is a way to organize safe conditions for the development of technologies, not a means to block technological development. At the same time, if envisaged

damage is considered sufficiently serious, then this may lead to the renouncing of specific technologies or specific applications, especially if less threatening alternatives are available at a moderate cost.

For EU law, which was constructed to promote the free circulation of goods, proportionality includes three key requirements (Gonzales-Vaqué *et al.*, 1999):

- the measure should be appropriate to its objective (notion of efficacy);
- the measure should be necessary in the sense that there are no other measures that are equally effective and less restrictive for international trade;
- there should be a reasonable link between the objective sought and the constraints imposed on the circulation of goods.

Within the national contexts of member states, other dimensions of proportionality are relevant. All costs and benefits that are potentially involved, including ethical considerations (basic liberties versus safety, for instance) must be examined for each measure and balanced with the possible seriousness of the damage. In this regard, due attention should be given to the extent and richness of the scientific basis supporting hypotheses of risks, in order to assess scientific plausibility in absence of reliable probabilities (Godard, 2003).

### 3.3. Burden of Proof

Whatever else has been said on this issue (Raffensperger and Tickner, 1999; Hansen *et al.*, 2007), the idea of shifting the burden of proof is not at the core of the EU's PP doctrine, but exists as an option that may be appropriate depending on the situation. For example, for food additives, new foods or drugs, the PP should simply be incorporated into existing administrative authorization procedures prior to products being released onto the market, without necessitating a change to pre-existing rules. For products and processes that are already on the market and in widespread use, the responsibility of providing the required scientific evidence to support the suspicion of harm rests with the third parties or public authorities that have raised concerns on possible unacceptable harm.

In fact, in the context of the PP, the idea of reversing the burden of proof is quite ambiguous and conceals a real shift regarding what has to be proven. Strictly speaking, shifting the burden of proof and demanding evidence to demonstrate absolute safety is a logical impossibility. The

scientific proof of the harmlessness of a product, substance or technique can never be definitive when the scientific knowledge it is based on is neither complete nor fixed and when it incorporates uncertainty. Numerous authors have emphasized this impossibility. Some sources of uncertainty may be reduced with research, experience and time; others reflect the intrinsic incompleteness of knowledge. Hence, while the PP demands an early consideration of risks, this does not equate to a shift of the burden of proof but instead to the movement of public risk management away from the concept of scientific proof, and maintaining the distance between them, whether proving damage or proving safety is the focus. Naturally, this does not mean that public management should ignore scientific knowledge. Rather, the contrary is true: the PP requires risk management to become more attentive to science in development and to what constitutes the ordinary course of research (conjectures, hypotheses, ambiguous results, etc.).

When they are anxious to remain intellectually honest, authors that speak of a reversal of the burden of proof confess that they do not in fact mean that the objective should be to demonstrate proof of the absence of risk, but that authorization procedures should be set up for industry or engineering firms to present results of studies establishing the safety of their products or technologies by using standard tests based on existing knowledge. Yet such tests cannot dismiss the possibility of future harm in relation to unknown developments. When activists ask for proof of the absence of risk, with a time horizon that extends to long-term effects, then this is quite a different thing. By insisting on something that scientists cannot deliver, they slide into mere political rhetoric and use the argument of reversal of proof as a means to obtain endless moratoriums against targeted products and technologies.

Moreover, assigning the responsibility of developing studies and safety tests to stakeholders with products and technologies that they want to put on the market is not the best means to ensure the credibility and transparency of scientific expertise on risks (Godard, 2005), even if such individuals are competent and honest. Knowledge acquisition on risks is expected to be independent and carried out transparently and according to precise multidisciplinary rules and the principles of adversarial examination and open debate. These conditions are not only difficult for private businesses to achieve, but whenever such expertise and information does come from the private sector, it is often met with public scepticism. So how can we ensure that information transmitted to public expert committees is not incomplete and truncated?

This reasoning argues in favour of a separation between the financial



burden of studies and the assignment of operational responsibility for scientific tests. The latter should be attributed to independent scientific applied research and tests should be conducted under public supervision and open scrutiny, which is not the case under the present EU regulations. The quality of the review process by public agencies is no substitute for the quality and credibility of primary studies on which public agencies depend.

### **3.4. Searching for Consistency, An Extension of a Comparative Approach**

The rationale of the PP is not to justify extreme and extravagant measures that would paradoxically be much more demanding and restrictive than those taken for well-documented and evaluated risks. Calling for policy consistency implies an extension of the perimeter of assessment to include similar cases and thus enabling comparative approaches. Profiles of several similar risks, some potential and others ascertained, should be compared. An analogous extension results from the consideration of potential precautionary actions, which could include less hazardous alternatives: due to knowledge and data limitations on the possible outcomes resulting from the introduction of new technologies or new products, attention may shift towards the search for substitutes with a priori lower impacts. In this regard some authors propose the substitution of a focus on risks (endpoints) by one on intrinsic features of hazards, from risk assessment to hazard assessment. For instance Müller-Herold *et al.* (2005) suggest the systematic consideration of the existence of amplifying factors able to transform local damages into large-scale ones, and to use them as filters in an authorization process. According to these views, the PP does not only call for the consideration of a whole spectrum of candidate actions to control a given threat of damage, but also to search for the existence of alternatives to suspected technologies or products and so avoid risk-risk tradeoffs (Hansen *et al.*, 2007).

### **3.5. Taking Risks to Improve Knowledge and Reduce Uncertainty**

Far from catastrophism, the PP should be able to accept activities suspected of creating health or environmental risks, even when such risks are poorly understood, but with progressive commitment and a special side-programme of observation in order to identify the first signs of emerging damage and to learn about the presumed risks. This is one of the

paradoxes created by the PP: it may be necessary to take risks in order to check the very existence of those risks and to gain knowledge of them.<sup>9</sup> This commitment is linked to the key conceptual component of the PP that refutes any complacent acceptance of initial scientific uncertainty: the PP should not be the ultimate rationale of risk management but the one that organizes the transition to a state of better knowledge of risks, allowing a move from precaution to prevention. The early stage consideration of risk hypotheses should be supplemented by specific programmes aiming at reducing and possibly eliminating this uncertainty. In this respect, the PP is different from the sort of instrumentalization of scientific uncertainty, which is used to service the interests of stakeholders who use debate on the management of potential risks to improve their social positions or power, or to achieve specific objectives.

#### **4. The Dead End of Catastrophism**

The PP calls for an early on account of the potential or hypothetical threats, in spite of any remaining scientific uncertainty. It also asks for proportionate and provisional measures. Is well thought-out precaution possible if done early? Are we not faced by a basic contradiction between the obligation to take early action and the search for cost-efficient action? If we want to prevent hypothetical risks translating into actual damage, are we not obliged to take measures based on the worst-case scenario, which would make no difference between known risks and potential risks, between prevention and precaution? All these questions revolve around the same issue: to control hypothetical risks, is it not necessary to embrace a catastrophist perspective?

In its full conceptual development, catastrophism can be characterized by the combination of three ideas (Godard, 2006): (1) tackling an uncertain context by focusing on the worst-case scenario; (2) deciding, by convention, to consider this scenario as certain if no action is undertaken;

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<sup>9</sup> Decision theory confronted with irreversibility has shown the existence of three types of irreversibility: those affecting the set of possible actions; those concerning the real consequences on the environment or human health; and those affecting future knowledge and information. Amongst the range of actions that can bring new information are those that generate uncertain risks. Forbidding them asks to renounce to valuable new insights on these possible risks or on other subjects. If the expected knowledge and information that such actions are anticipated to provide is judged important, then the best choice may be to commit to the potentially risky action that will deliver such information.

and (3) choosing the forms and intensity of preventive action necessary to block the realisation of this scenario.

There are several types of catastrophism, ranging from the most respectable philosophical work of Hans Jonas (1984) to confused, ordinary and inadvertent ones. None are defensible since all are stricken by theoretical inconsistency or nonsensical arguments.

#### **4.1. Catastrophism and Hans Jonas's Responsibility Principle**

The start point of Hans Jonas's thinking is the consideration of the huge threat that the power of modern technology poses for the future existence of humanity. Hence, Jonas puts forward the idea of a new responsibility for the future. Jonas also holds a specific view of technology: technology is only controllable in its beginnings and in the first steps of development and diffusion; subsequently technology spreads throughout society and becomes an autonomous, unmanageable force. Action to control technology at its beginnings is the only way to safeguard the future of humanity from anticipated catastrophes. In order to be well adapted, control of technological impacts should be based on scientific forecasting<sup>10</sup> but also on the mobilization of imagination and sensitivity to develop awareness of possible future consequences of technology. This is what Jonas calls the "heuristics of fear". What is important for him is for technologies that may have direct and indirect apocalyptic impacts on the existence of humanity to be clearly distinguished from all other technologies. Avoiding apocalyptic risks is, according to Jonas, the sole and unique moral categorical imperative: such risks must be eliminated, whatever the probabilities involved and whatever the expected benefits of the technological development under scrutiny. In this regard, reversing the Cartesian position,<sup>11</sup> the mere possibility of an apocalyptic risk should be considered as a certainty at the moment of profiling prevention measures intended to eradicate these types of risks. For non-apocalyptic risks,

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<sup>10</sup> Jonas underlines the new moral status given to what he calls "futurology", a future-oriented science dedicated to the identification and assessment of possible effects of technological developments in relation to the environment and human essence.

<sup>11</sup> Jonas wrote: "To establish the indubitable truth, we must, according to Descartes, hold everything that in one way or another may be put into doubt as equivalent to a proven falsehood. Here, on the contrary, we must treat that which can certainly be put into doubt, as long as it is possible—once we're dealing with a possibility of a certain kind—as a certainty with respect to our decisions". Here the "possibility of a certain kind" referred to an apocalyptic outcome.

ordinary risk management considering costs and benefits of technology is acceptable, which would allow for the possibility of some damage becoming reality: individuals have the right to put their own existence at risk, but not the right to put the existence of humanity at risk. According to the heuristics of fear, if a technology incorporates a chance of causing apocalyptic harm, even indirectly or far ahead into the future, it should be rejected and banned.

The value of the new maxim depends on the capacity of risk managers to ascertain at an early stage which technologies are potentially apocalyptic and which ones are not. If the possibility of apocalyptic outcomes cannot be dismissed on the basis of scientific investigations, it should be categorized as “certainly apocalyptic” according to Jonas. This position is flawed and reveals inner contradictions in the thoughts of Jonas. The structural incapacity of scientific knowledge to embrace the full spread of potential effects of a technology, on which Jonas bases the argument in favour of his “heuristics of fear”, means that the possibility of an apocalyptic outcome can never be ruled out. Since Jonas excludes any reference to the idea of probability, all technological developments can be said to be potentially apocalyptic, whatever the level of plausibility involved (Godard, Lagadec, Henry & Michel-Kerjan, 2002; Godard, 2003). And therefore any technological development should be banned at its outset because of these risks.

Through the application of his formal distinction between apocalyptic and ordinary risks, the Jonas maxim would cause a paralysis of human action. Even if we can accept many of his premises, the model of action he puts forward leads to a logical and practical dead end. Furthermore, this radical conception would give rise to a false sense of security, since a paralysis of innovation would leave humanity in the dependence of existing technologies, whereas many of these technologies were at the source of the present environmental crisis. The PP should definitely put aside the “guilty if not proven innocent” position inspired by Jonas, since innocence can never be proven.

## **4.2. Ordinary Catastrophism**

There is not much to say about ordinary catastrophism, which is simply an extension of Jonas’ maxim to apply to all possible threats to the environment and human health, an extension that Jonas considered as highly irrational. The aim of the PP cannot be to eradicate at source any possible risk. It remains anyway a meta-decision process of choosing between potential risks that can be taken, accompanied by proportional

and provisional precautionary measures having to be regularly revised in view of experience and the progress of knowledge, and those potential risks that should not. Such meta-decisions cannot be taken by applying the general mantra of reversed proof of safety.

A weak form of ordinary catastrophism is to call for policy choices that minimize the possible damages caused by a range of technological options, with no consideration given to costs and scientific plausibility. Inspired by John Rawls, although in relation to a different subject, Gardiner (2006) has defended this so-called *maximin rule* as the core PP. The justification brought underscores specific contextual features: no credible probability can be ascertained, potential gains are negligible where compared with plausible potential harm, and alternative courses of action all give unacceptable outcomes. These are very particular conditions and certainly not a general model of situations calling for the management of uncertain risks. Furthermore the value of this rule vanishes in contexts where all possible outcomes have not been identified and it is impossible to define a closed set of outcomes. In the latter case, the *game space* is not fixed and the logic of the maximin rule cannot be applied. It will only result in indecision because the *race to the bottom* will ensure the equalization of all options by equally unacceptable catastrophic worst possible outcomes: what course of action should you take if the possible end-result of all alternatives is apocalypse?

### **4.3. Involuntary Catastrophism: The Earliness-severity Artefact**

There is a certain type of risk assessment, apparently supported by ethics or common sense and goodwill, which triggers an involuntary catastrophism. This occurs because of a pure artefact that results from an inverse relation between the promptness of the consideration of hypothetical risks and the possible seriousness of hypothetical harm (Godard, 2003, 2006): the initial justification of the PP is that the high level of severity and irreversibility of possible damage resulting from suspected risks provides the justification for early preventative action. The inverse relationship is that because considering risks at an early stage of knowledge development, i.e. when knowledge is still very poor, any risk may be suspected of potentially having apocalyptic consequences and then deserves the strongest prevention measures. This artefact may impose itself whatever the empirical nature of the considered sources of risk. The underpinning logic is that the earlier on a risk is considered in relation to the level of scientific knowledge, the greater the number of hypotheses and

conjectures there will be that have not yet been proven wrong, and so the set of possible scenarios under consideration will include having certain serious outcomes and others really catastrophic ones. Thus the envisaged technology will be perceived as highly dangerous, which in turn will call for severe restrictive measures. This result being obtained for any technology considered at its very beginning, one then ends up with the same aporetic result as Jonas's maxim.

The biased assessment procedure giving rise to these unexpected aporetic effects rests on two statements that are regarded as "axioms" that at first glance look attractive. The first requires that the public appraisal of a collective risk only consider possible damages, without looking at the possible benefits for society. The underlying rationale is that the principle of basic entrepreneurship freedom assigns entrepreneurs with the responsibility of appraising the benefits of their own projects or technical innovations and bearing the economic risks of their endeavour; public responsibility is thus limited to making sure that these initiatives do not generate unacceptable damage for society.<sup>12</sup> The second axiom is basically similar to Jonas's position, in that it requires, for the sake of the future, that a non-invalidated possibility should be treated as a certainty. The combination of these two axioms is sufficient to trigger the earliness-seriousness artefact.

To avoid this deleterious artefact it is necessary to reverse the content of the two axioms. First, risk assessment should also take into account the various social benefits of technical developments, without confining itself to potential damage. Next, it is essential to differentiate risk hypotheses according to their degree of plausibility and scientific consistency: a hypothesis that lacks any empirical and theoretical support should not be treated in the same way as a hypothesis that is strongly supported by scientific inputs but that has still not been established according to the views of a majority of competent scientists.

## 5. The Specifics of Chemical Risks

Chemistry is an "impure science" since it intrinsically combines the quest for knowledge with technological applications. As Bensaude & Simon (2008) put it, "chemistry serves as the archetypal techno-science,

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<sup>12</sup> This principle does not apply in the area of drugs and medical products where, on the contrary, risk-benefit analysis has been adopted by medical circles as the best assessment framework. But in this case, benefits as well as risks of damage are related to health impacts and do not directly embrace the commercial benefits for drug companies.

unable to restrict itself to the high-ground of pure theory, but always engaged in productive practice.”

The industrial production of chemicals has been a major new source of environmental disruption since WWII, allowing for the industrialization of agricultural production by the intensive use of energy and chemical inputs and also for the mass usage of plastic products and packaging (Milton & Farvar, 1972). Pesticide residues have come to the forefront as a huge threat to human health through the contamination of food, and we find traces of industrial chemicals in every water sample taken throughout the world. Given the pervasive diffusion of chemicals, it is all the more striking that most substances have not been appropriately tested for their environmental and health impacts beyond light toxicity tests. This element of the unknown is not a feature that is unique to new molecules that chemistry has recently invented; it is the most common feature of chemicals that have already been disseminated into the atmosphere, waters and soils for several decades. The threat has already existed for some time, and we have known little of it. With regards to these threats, the early on ascertainment of risks was far from the reality.

Another feature of chemistry as a science is that it produces new substances and not only knowledge on the existing material world. New substances introduce new properties that are difficult to anticipate, with possible consequences that are difficult to fully comprehend. So, development in chemistry is a permanent source of new unknowns. Today, biochemistry brings the new challenge of the creation of synthetic life. The heritage of the alchemical dream remains. As said by Schummer (2001), “With every production of a new substance, the scope of nonknowledge increases tremendously, by the number of undetermined properties of the new substance as well as by all chemical reactivities of the already existing substances with the new one.”

Due to the massive number of new chemical substances that are being introduced into ecosystems, this creative process entails an increasing unpredictability of environmental changes. The creation of a new substance and putting it on the market generates a new unpredictable potential for harming the environment and public health, increasing the difficulties associated with the control of these harms. This is a legitimate source of concern: chemistry is a major factor in making our world unpredictable. There is no better justification for submitting products derived from innovation in the field of chemistry to rigorous procedures of public control, and to place these procedures under the flag of the PP.

## **6. REACH and Chemicals**

### **6.1. An Outline**

Following a 2001 White Paper, the European REACH (Registration, Evaluation and Authorization of Chemicals) regulation came into force on 1 June 2007. It was the result of a chaotic six-year deliberation process that was stimulated by markedly opposing opinions on how to strike a balance between public health, environmental quality and industrial competitiveness. Elizabeth Fisher (2008) saw in that process a “perfect storm” due to the convergence of three components: a radically innovative approach regarding new information duties of business, both in bearing the burden of safety studies and in disseminating information to all stakeholders alongside the supply chain; the rewriting of the conditions of access to the market by making registration an absolute condition to obtain a “licence to operate” in order to achieve sustainable development; and the spread of impacts on multiple jurisdictions within and outside the EU.

This regulation echoed several concerns in relation to, respectively, the health and environmental impacts of toxic substances, the lack of knowledge about the effects of most chemicals that have been put onto the market and disseminated into physical environments, the incapability of governments to inform and run timely controls of thousands of chemical substances, and last but not least, the lack of incentives for safer and greener chemicals due to the previous regulation’s focus on new substances from 1981.

The REACH regulation consists of three main components:

1. Registration of all chemicals (substances and products) intended for the market, be they “new” or “old”, provided that their level of production exceeds 1 tonne/year/producer. The procedure asks producers and importers to provide information for the identification of substances in terms of properties and usages and to specify envisaged levels of production and sales. For substances produced or imported in quantities of more than 10 tonnes/year/producer, a chemical safety report must be provided that gives the results of toxicity tests and defines appropriate management measures suitable for guaranteeing safe use. In particular this document should test the persistent, bioaccumulative and toxic (PBT) characteristics of substances and products. In this case, information needs are reinforced by the requirement for an exposure assessment and a risk characterisation.



2. Evaluation is conducted by member states according to guidelines and criteria elaborated by the new European Chemical Agency. It is required to check the quality of the testing and data that manufacturers deliver and also to determine which regulatory status is given to candidate chemicals. Specific attention is given to substances and products that should be classified as dangerous. On the basis of their evaluation, member states present proposals of classification to the European Agency, which examines them with the help of three committees (risk assessment, socio-economic and member states) before making final proposals to the Commission.
3. The authorization of chemicals is based on evaluation. Specific authorization is assigned to a chemical depending on the level of danger and the quantities involved. Restrictions or complete bans on certain chemicals may result if they cannot be used safely and their usage is not essential. A key point is that producers must establish whether it is possible to use their chemicals safely. Dangerous products will not be authorized due to their lack of safety, unless it can be demonstrated that the benefits for society are higher than possible harm to public health and the environment. In these instances, authorisations with restrictions in scope and time may be granted.

The initial deadline for the registration of chemicals was November 2010 for chemicals produced in quantities of more than 10,000 tonnes/year. 4,300 substances were registered before this deadline. Deadlines for other categories are forecast for 2013 and 2018. Priority for examination and decisions on authorisation has been given to substances of very high concern (persistent, bioaccumulative, toxic, mutagenic, carcinogenic or reprotoxic).

## **6.2. An Assessment in the Light of the PP**

REACH has often been presented, especially by the Commission (Rogers, 2003; Fisher, 2008), as an application of the PP in the specific field of the use and dissemination of chemicals. It is true that article I(3) of the REACH regulation presents the new rules as being “underpinned by the precautionary principle”. At the same time, the supporters of radical conceptions of the PP, such as Hansen et al. (2007), have expressed their doubts on the precautionary content of REACH.

These authors express regret that REACH refers to the 2000 Communication of the Commission, which in their eyes is not a correct

expression of the PP because: a) it adopts an overly restrictive understanding of scientific uncertainty, as if scientific research and improvements in scientific methods will suffice to make them disappear; b) it sets the PP in the framework of a standard risk assessment and confirms the separation between risk assessment and risk management in spite of the pervasive presence of value judgements in risk assessment, what is generally called the “framing of expertise”; and c) it expresses a defensive and reactive approach, filtering technologies and products but insufficiently promoting the search for safer alternatives. Regarding REACH, they regret that the regulatory authorities have to demonstrate the existence of a risk and provide proof of the indications of its severity before they can decide on any restrictions. This requirement imposes the burden of proof on the shoulders of public bodies, which is contradictory to the perceptions of the PP held by these authors. They acknowledge the shift of responsibility for the collection of data and the performing of tests, but consider this insufficient for a full implementation of the PP. Lastly, they regret that the involvement of stakeholders is not systematic at the different stages of registration, evaluation and authorisation, and the opportunity for the public to comment on risk assessment and socio-economic analyses is not precisely linked with the decision-making process.

I suggest a more balanced assessment. Several features fit well with the PP’s rationale. First REACH confirms that we do not have to be afraid of uncertainty. Uncertainty is not a legitimate motive to postpone safety regulation. It is possible to discriminate between chemicals on the basis of an evaluation considering a mix of possible impacts and inherent characteristics of substances. It is clear that chemicals are exposed to regulation before any harm is observed, confirming the PP’s focus on early action for new substances. It is then necessary to remain alert to avoid both false negatives and false positives since, as Vlek (2010b) puts it, “the required level of evidence for precautionary action cannot be fixed but should depend on the prior probability or plausibility of harm and the seriousness of possible false-positive versus false negative decision consequences” (p. 564).

Secondly, similarly to the PP, REACH reaffirms the key role of scientific expertise for evaluating the riskiness and safety of chemicals. Regulation is not expected to disintegrate with the quest for scientific objectivity, but to be based on the soundest scientific assessment possible and to be submitted to the comments of stakeholders.<sup>13</sup> REACH also

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<sup>13</sup> To keep up with the values of rationality and consistency in overall safety policy, it is important not to downgrade the contribution of scientific investigation, and to fight against an increasing tendency to design policy responses on the basis

shows no complacency towards uncertainty, since the bulk of this regulation is to oblige businesses to gather and share huge amounts of data relevant for safety. Thirdly, in spite of the principle that the safety of a substance has to be established in order for it to be authorized, REACH does not fall into the trap of catastrophism since in cases where a chemical product is difficult to substitute and generates important benefits to society, a balance of threats and benefits has to be achieved, which demand subsequent regulatory treatment. This is a partial echo of the core idea of proportionality.

This being acknowledged, it is fair to say that the main purpose of REACH is not to implement the PP. By and large REACH belongs mainly to the universe of prevention based on the proof of safety concept, just like the 2002 Regulation on food safety, and on standard tests and stabilized science in toxicology and other related disciplines. These tests are very useful for understanding direct harm on human health, but are not as well designed to ascertain new effect types or systemic environmental risks, such as those affecting biodiversity or human health through chemical synergies between various trace substances (Maxim and Spangenberg, 2009). In this regard, there is a search for proxies and alternative procedures based either on the inherent characteristics of substances, amplifying factors of damage or determinants of scale (extent and dissemination of the demand for products, safely confined versus open use, etc.) in order to identify filters, thresholds and screening conditions (Klinke et al., 2006) by non arbitrary methods.

Another area of divergence with the PP is the shift to industry of the operational burden of studying environmental and health impacts of chemicals and getting primary data on safety. This is a risky gamble from the viewpoint of the scope and the quality of studies since the short-term drive for profit may mean that businesses do not conduct as many investigations and tests as would have been made under public control, and nor will they transfer all of the relevant information to public authorities and other stakeholders, including consumers and the public. Furthermore, there is an issue of credibility: it is not possible to have companies conducting or controlling safety studies in the name of responsibility, while at the same time calling for independent, pluralist and transparent expertise on risks, as is required by the PP. It is certainly

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of political tactics, in response to green NGO activism or to other lobbyists, as shown by Nilson (2004) for chemicals in the case of Sweden, or by Godard (2011) for GMOs in the case of France. Socio-political contexts and their consequences on decision-making are well analysed by Sunstein, (2005) and Lofstedt *et al.* (2011).

useful to involve businesses in the management of risks imposed on society, but the PP certainly demands a more diverse source of studies and data than those disseminated by companies with an interest in placing their own products onto the market. Secondary assessment and checks by public agencies can be no substitute for the control of primary sources of information and the steering of the primary impulse of focused scientific research.

A last point concerns the conception of the regulation. The PP puts forward a new philosophy of preventive action that conceives precautionary measures as provisional, flexible and attentive to the development of empirical and scientific knowledge, without inflicting irreversible commitments or irreversible prohibitions on future citizens and decision makers; such measures should be periodically revised accordingly. REACH does not fit well with this fluid approach to precautionary actions,<sup>14</sup> since its aim is to obtain quasi once-only classifications of substances and, for the supposedly more dangerous ones, to decide on their definitive exclusion. This is understandable given the massive number of substances requiring registration and evaluation, and the necessity to make up for years of negligence regarding the impact of chemicals already disseminated into the environment. Therefore, a specific and distinct role should be maintained for the PP in the field of chemical regulation, in parallel to REACH.

## Conclusion

Although the PP was introduced into the European landscape twenty years ago, its content is still fiercely debated. Discrepancies between concepts and between concepts and achievements are striking. In spite of an absence of consensus, in 2000 the EU adopted a public doctrine of the PP, which stands as a valuable landmark for a “reasonable” and “proportionate” management of hypothetical risks. Earliness, proportionality and the reversibility of precautionary actions thus strongly demonstrate that the PP does not embrace a catastrophist viewpoint.

Chemicals are of prime importance in the quest to raise safety standards for environmental and human health because of their specific and novel features. As a discipline, chemistry is a permanent source of new unknowns, which justifies special attention being paid to the risks it potentially raises. In Europe the REACH regulation has important

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<sup>14</sup> It should be noted that this is the component of the PP that the case law of the European Court of Justice tends to disregard (Rogers, 2011).

elements in common with the PP, such as the necessity to take action without waiting for full scientific certainty and a reliance on scientific expertise to enlighten policy choices in parallel to consultations with stakeholders. At the same time, the huge shift of responsibility for producing the relevant risk data onto companies with direct interest in putting their own products on the marketplace is a source of tension with the PP requirement to set up an independent and transparent knowledge base, remote from vested interests. REACH is also much more rigid than is expected from precautionary actions under the PP.

All this suggests that the PP should continue to play a trusted role alongside the larger administrative programme of the registration and evaluation of chemicals driven by REACH. In this regard the PP should serve as a guiding light to enlighten developments in green chemistry. Researchers from a wide range of backgrounds are encouraged to help meet the challenge of developing a nice regulatory regime based on the PP, one that strikes a proper balance between the enhancement of chemical innovation for sustainable development and the timely control of potential risks associated with emerging technologies and products.

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# THE LIMITS OF MODERN CHEMICAL ANALYSIS: METROLOGICAL AND EPISTEMOLOGICAL INSIGHTS

STÉPHANE BOUCHONNET AND SAÏD KINANI

## Introduction

Analytical chemistry is omnipresent today: it is used in molecular biology, medicine, pharmacology, toxicological investigations, the petrochemical industry, agro-industrial, atmospheric and environmental analysis, and in the inspection of industrial production. The discipline borrows methods from various sciences: organic chemistry (e.g. for preparing samples), chemical physics (i.e. for chromatographic, spectrometric and spectroscopic techniques) and mathematics (i.e. for experimental design and the statistical treatment of data). Analytical chemistry is undergoing constant change and in recent years has seen both a extensive improvement in existing techniques—such as solid-phase extraction, which has experienced spectacular progress (Poople, 2003) — and the emergence of new techniques, such as ionic mobility combined with mass spectrometry (Kanu *et al.*, 2008) and the orbital ion trap (Scigelova & Makarov, 2009), which applies innovative concepts.

Unlike other experimental sciences, analytical chemistry currently attracts a very large number of students, probably for two main reasons. The first is that it offers jobs at all levels of qualification, in a wide variety of business sectors, both within small- and medium-sized companies and international industrial corporate groups. Ever stricter health inspection standards, the rise of the precautionary principle and quality labels (e.g. ISO and AFNOR standards) all contribute greatly to employment opportunities in this field of chemistry. The other reason for the success of this discipline with students is undoubtedly its huge presence in the media. We have lost count of the number of films and TV series featuring police forensic experts (to varying degrees of relevance) and the plethora of

documentaries and press articles dedicated to the problems of environmental pollution and to enquiries into the quality of our food.

In spite of its spectacular developments and all the strategies deployed to come close to reality as defined by David Hume in his *A Treatise of Human Nature* (2000), analytical chemistry is frequently confronted with metrological, methodological and epistemological questions. We will not cover here the economic problems resulting from the globalisation of the analyses or ethical and social problems posed by the application of different standards in different parts of the world. We will be dealing with a number of scientific questions with which chemists are confronted. Some of these questions, inherent in the methodology itself, may appear unanswerable, so that we might ask ourselves whether certain of the method validation protocols currently in force have not reached their limits.

We will briefly describe a methodology traditionally used for developing and validating a method in analytical chemistry before dealing with the aforementioned problems through several examples of analytical methods with metrological, methodological or epistemological limitations. We are thus inviting philosophers to look into these questions we face as analytical chemistry professionals, in hopes that they might throw light on them from a new angle, contributing to an area where most debates about analytical standardisation involve experts exclusively from the scientific world (chemists, biologists, statisticians, etc.).

## **1. Traditional Methodology for Developing and Validating an Analytical Method**

There is no universal methodology for the development of analytical chemistry methods, still less a standard validation protocol. Here, we are talking about simply describing the various steps involved in a titration method for one or more compounds in a given matrix and the sequencing of these steps in order to gain a better understanding of the difficulties described in the following paragraphs. In analytical chemistry, the term 'matrix' describes the substrate, the medium in which the molecules to be characterised and titrated are located (e.g. biological fluid, foodstuff, vegetable matter, cosmetics, river water). It is generally an extremely complex medium within which the molecules we want to analyse are subject to a multitude of interactions with those surrounding them.

### **1.1. The Main Steps of a Titration Method in Analytical Chemistry**

In the most recent methodologies, an analysis consists of at least three steps: taking the sample, preparing the sample and carrying out the physicochemical analysis. The sample may be collected in a number of ways. Generally, plastic, glass or metal containers are used to gather samples of water (river, lake, ocean, tap water, etc.), sand, earth, sediment or vegetable matter for environmental analysis. Blood is sampled using a plastic syringe, and urine and milk using sterilised flasks made of Pyrex or, most often, plastic, for medical, pharmacological and veterinary analyses.

The second step is usually called ‘sample preparation’. Its main objective is to extract the analytes from the matrix. The techniques traditionally used are liquid–liquid extraction and solid-phase extraction for liquid matrices, Soxhlet liquid–solid extraction, extraction under pressurised fluid(s) and microwave-assisted extraction for solid matrices. Extraction is generally accompanied by a reconcentration of the sample, which aims to reduce the detection limits of the method. Reconcentration factors between 10 and 1000 are frequent. The preparation of the sample often includes a purification step whose purpose is to increase the selectivity of the analysis by reducing interferences with matrix compounds. It may also include a chemical derivation step of the analyte(s). Chemical derivation consists in chemically modifying the molecule to be analysed by making it react with a given reagent to enable or to improve chromatographic separation or detection by mass spectrometry. For example, a carboxylic acid may be converted into a methyl ester after reaction with methanol. The methyl ester thus formed is much easier to titrate by GC–MS than the corresponding acid, as the chromatographic peak relating to an ester is generally finer and more Gaussian than that of the corresponding acid.

The third step in the analytical protocol is the use of a physicochemical method for the detection and quantification of the analytes. The techniques mainly used today for the analysis of organic molecules are Gas Chromatography coupled with Mass Spectrometry, or ‘GC–MS’, for volatile or easily volatilizable molecules, and Liquid Chromatography coupled with Mass Spectrometry, or ‘LC–MS’, for less volatile molecules (polar molecules, salts, compounds with high molecular weight, etc.) These techniques are gradually replacing ‘traditional’ chromatography techniques such as high-performance chromatography with UV detection or gas chromatography with a flame ionisation or electron capture detector. They are becoming more and more widespread as they allow the

simultaneous titration of dozens of molecules in trace amounts in a few minutes. Nuclear Magnetic Resonance (NMR) techniques are more powerful in terms of structural characterisation but require larger samples, which is not compatible with trace analysis. Furthermore they require the sample to be extremely pure, their combination with a separation technique being still at the development phase.

If we exclude non-scientific criteria such as the cost of an analysis, its duration and its ease of implementation, the performance of an analytical method is characterised by three criteria: its specificity, selectivity and sensitivity. The specificity of the method is expressed by its ability to titrate unambiguously the analytes for which it has been programmed and not those molecules which resemble it. We say that a method is selective when the presence of interferences in the matrix does not affect the result of the titration. The sensitivity of the method increases with its ability to determine ever-lower analyte concentrations (it is more rigorous to talk of the detection or quantification limit) (Bouchonnet, 2009).

It should be noted that when the method is being developed, steps 2 and 3 are reversed, i.e. the physicochemical method (GC–MS, LC–MS or other) is optimised before the development of the sample preparation process since the tool is needed to evaluate the efficiency of the sample preparation protocol in terms of extraction efficiency, repeatability, selectivity, etc.

## 1.2. Validation Concepts

Prior to carrying out any titration, the analytical method has been calibrated and validated for each of the analytes. Calibration involves plotting what we call the ‘response function’, the relationship—often linear but sometimes quadratic—between the chromatographic response of the analyte (area of the chromatographic peak of the analyte divided by the area of the chromatic peak of an internal standard specimen) and the concentration of the analyte in the test sample (figure 1). The presence of an internal standard specimen is absolutely essential for correcting the innumerable sources of errors inherent in the preparation of the sample as well as in analysis by GC–MS or LC–MS. It is also of prime importance to plot the response function using the analysis of samples from the reference matrix (‘blank’ matrix, i.e. one which is uncontaminated, or a certified reference material) doped with known concentrations of analytes. In this way, the samples used to plot the function are all subject to the analytical protocol from beginning to end (including preparation of the sample), as the samples subsequently to be titrated will be. The ‘matrix effects’—

effects that may be attributed to all the molecules in the matrix interfering with the analytes—are thus taken into account in the calibration of the method.

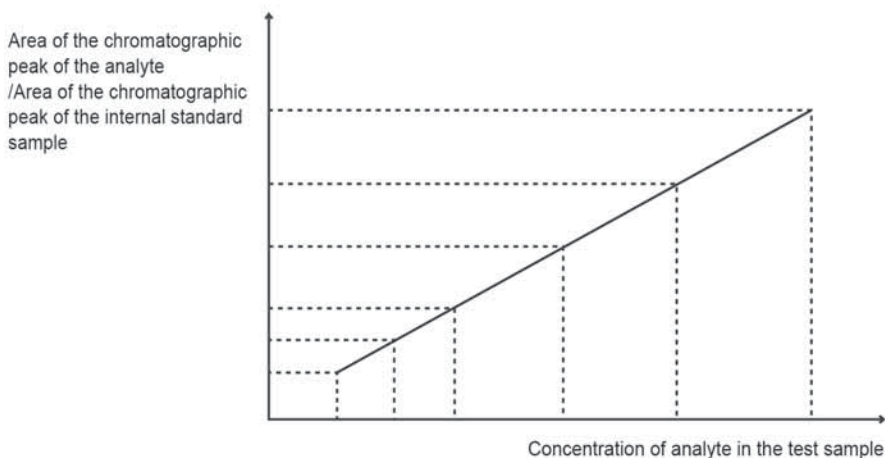


Figure 1. Response function of the analytical method for a given analyte.

With the response function determined, there are several approaches for validating the method, the most widespread being to analyse the so-called ‘quality control’ samples, samples of the reference matrix doped with known concentrations of analytes and standard specimens. At each of these levels of concentration, between the quantification limit and the maximum concentration that can be titrated, we check the accuracy, repeatability (accuracy of the measurements over one day) and the intermediate trustworthiness (accuracy of the measurements over several days) for the method. Depending on the field of application of the method, we test other parameters such as the stability of the samples over time, the effects of diluting the samples, etc.). The robustness of the analytical procedure will also be assessed. This expresses its ability not to be affected by small changes and free from factors associated with the procedure and thus gives indications as to its reliability. We could study, for example, the influence of the laboratory temperature, the pH of the matrix, the replacement of a worn part of the mass spectrometer, etc.

## 2. Problems Associated with the Relevance of the Reference Matrix

As recalled in paragraph 1.1, the use of a reference matrix is absolutely essential to the optimisation and validation of a titration method. The ideal reference matrix is clearly that which has the same structure and same composition as the samples to be subsequently routinely analysed. The absence of a suitable reference matrix is a recurrent problem in analytical chemistry. This problem is illustrated by means of three examples given below. The first is based on the development of a method dedicated to the titration of pesticides in green salad vegetables; the second describes the titration of cocaine and its main metabolites in the blood; the third deals with the development of a method of analysing PAHs (Polycyclic Aromatic Hydrocarbons: naphthalene, anthracene, etc.) in river sediments. We will also cover at the end of this section the problems posed by the deterioration of samples during storage.

### 2.1. Titration of Pesticides in Green Salad Vegetables

We now consider the case of a method dedicated to the titration of pesticides in green salad (Zhang *et al.*, 2007). The chemist is confronted by two problems. The first is the difficulty of obtaining a matrix that we can be sure is ‘blank’ or ‘fresh’, i.e. free of any contamination by one of the molecules to be analysed. It is out of the question to take a salad vegetable from a grower: we would have no guarantee that it had not been treated and contains no pesticides. It goes without saying that, if this were the case, the calibration of the method would be distorted by the pesticides in question. A possible solution would be then to take a salad vegetable cultivated under glass under ‘organic’ conditions. Proceeding thus, we make the assertion that this vegetable will show exactly the same characteristics as those cultivated ‘industrially’ which are to be analysed after the method is validated, which is not necessarily the case. The optimised extraction protocol may therefore prove to be inadequate. We could nevertheless assume that the textures and chemical compositions of the salad vegetables considered will be ‘sufficiently’ near for the extraction of the analytes to be repeatable between the reference matrix and actual samples or at least the use of one or more internal standard specimens will compensate for the discrepancies. This remains a hypothesis.

Beyond the question of the ‘blank’ character of the reference matrix is the question of its representativeness. Can a method validated for titrating pesticides in lettuce be used for titrating the same pesticides in other

varieties such as Batavia, romaine, curly endive, escarole or lamb's lettuce? By extension, can it be used to analyse spinach, chicory or cabbage? No, as there exists what we call a 'matrix effect', namely that the various components of the matrix substrate interact with the analytes during the preparation phase of the sample or during the physicochemical analysis. When the make-up of the tissue is modified, these interactions are also modified. Thus an analytical method is applicable only to the matrix for which it has been validated. A laboratory titrating pesticides in vegetables should therefore 'in theory' have validated a method for each variety of vegetable with which it is faced. Not only is this technically extremely tedious, but it is not very compatible with the specifications of an analytical laboratory in terms of cost. So laboratories generally use the same method for analysing the various salad varieties.

## **2.2. Titrating Cocaine and its Principle Metabolites in Urine**

Let us now consider a method for titrating cocaine and its principle metabolites in human urine. If the question of the 'blank' character of the matrix does not present a problem in this case (we can still easily find people who do not take cocaine!), that of its representativeness is more complex (Janicka *et al.*, 2010). Indeed, the chemical composition of urine (even its pH) is complex and can vary considerably from one individual to another. We will therefore generally need to use what we call a urine 'pool', a mixture of urines from individuals of different ages, sexes, body weights and if possible lifestyles (Mazzarino *et al.*, 2011). This urine pool constitutes the least worst solution to the problem of representativeness of the matrix but even if this solution was practical and in principle adapted to the largest number of individuals, it is unsuitable for any analysis as the pool is not an 'actual' matrix in the sense that it is not a matrix which exists in nature, it is a 'model' giving the average of the possible situations. To be completely legitimate, the method would have had to be validated on the 'blank' urine from the patient, which could hardly be considered in clinical toxicology and would be completely impossible in emergency medicine or medico-legal investigations.

Note that although the blank character of the reference matrix is not a problem with cocaine, this is not true for all molecules relevant to toxicology. For example, we have recently found out that heroine or certain of its metabolites can be present endogenously at low concentrations in the blood following a significant amount of stress. It would therefore be necessary to check for the absence of heroine and its metabolites in the reference matrix before starting validation of the

method. The paradox of this situation is that it would be necessary to carry out this check with the method that would not at this stage have been validated!

Let's return to titrating cocaine and its principle metabolites in urine. The analysis becomes considerably more complex in legal medicine. Biological fluids degrade post-mortem, their composition and physicochemical properties change continuously. If urine is withdrawn from the bladder of a cadaver found ten days after death, its composition will not be the same as urine taken from a person who died the previous day or that of a living being. The jurist does not have reference urines to cope with all situations. Thus the method is generally validated with a reference matrix identical to that used in clinical toxicology. Not only will the sample preparation protocol not be perfectly suited to the matrix of the sample to be analysed but as the matrix interferences are not the same as those in the reference matrix, the 'matrix effects' caused by these interferences will be different in nature and intensity from those with which the method was validated (Gergov *et al.*, 2009).

When clearly an ideal reference matrix does not exist, the solution that naturally springs to the mind of the chemist is to use several internal standard specimens added to the test sample to compensate for the problems of extracting the analytes and the matrix effects. Given that the ideal standards are products marked with stable isotopes and that it would be advisable in theory to add as many as there are analytes to titrate, it would seem very difficult to envisage carrying out an investigation at a 'reasonable' price, above all when we know that toxicologists are often confronted with multiple intoxications involving a large number of toxic substances and the metabolites from these (Carson, 2008).

### **2.3. Titrating Endocrine Disruptors in River Sediments**

We have recently been faced with the development of methods using gas and liquid chromatography coupled with mass spectrometry to titrate dozens of endocrine disruptors (dioxins, chlorophenols, hydrogenated polyaromatics, oestrogens, etc.) in river sediments (Louiz *et al.*, 2008; Kinani *et al.*, 2010). In addition to the difficulties inherent in the development of so-called 'multi residue' methods aimed at titrating a large number of molecules with very varied physicochemical properties (difficulties in extracting all the analytes of the matrix while maintaining selectivity with regard to the matrix interferences), the problem of the absence of a reference matrix has a special significance. In this example we again meet the two types of difficulties mentioned above with regard to



the validation of the method: the absence of a 'blank' matrix and the problem of a representative reference matrix.

It is indeed impossible to obtain a 'blank' river sediment, i.e. one that we could be certain was not contaminated by any endocrine disruptor as this type of pollution affects the whole of the Earth's surface including the polar ice! (Trenholm *et al.*, 2006)

In addition, a sediment extracted from one river cannot be considered as representative of sediments from other rivers. The particle size distribution as well as the composition in organic materials and minerals varies considerably from one river to another and even between two sites of the same river.

The solution adopted by most laboratories certified for this type of analysis is to turn to a reference matrix which is a sediment 'artificially' reconstituted from peat, sand, etc. in precise proportions (Peng *et al.*, 2006). A standard sets these proportions and lays down how the reference sediment is to be prepared. The latter has the advantage of standardising the method validation between various laboratories and allows results to be compared between them. However, the criticism that could be levelled at the reconstituted sediment is that it does not relate to any 'actual' sediment. Clearly, its composition does not relate to that of a sediment rich in humus or of a very sandy sediment. Consequently, although this pragmatic solution allows results between different laboratories to be compared and to cut short disputes between experts, it is unsatisfactory in terms of the representativeness of the reference matrix and therefore not totally suitable for producing a model that aims to establish a satisfactory correlation in a precise empirical context. Furthermore, creating a sediment contaminated with optimum interactions between contaminants and sediment components requires the natural conditions under which the sediment is contaminated also to be simulated. Thus the water column in contact with the sediment needs to be doped, then agitated, aerated and given time for the interactions to occur. The main problem with this method lies in the fact that the extraction yield is always less than 100%. Determining the concentration by carrying out a mass balance is incorrect, part of the matter being systematically lost by transformation, deterioration or evaporation during the sediment preparation protocol.

## **2.4. Problems Posed by the Deterioration of Samples during Storage**

It may happen that the stability of the samples to be analysed poses a crucial problem, particularly with biological samples. During a toxicological

investigation undertaken as part as a legal or anti-doping enquiry, part of the sample is frozen in case a counter investigation is required, the latter taking place generally several weeks to several months after the initial analyses. Now we know perfectly well that freezing significantly modifies the physicochemical properties of biological tissues, as anyone who owns a freezer will readily testify (Soyer *et al.*, 2010). Even storage at very low temperatures ( $-80\text{ }^{\circ}\text{C}$  for the freezers currently in use in biology) does not stop the physiological changes in tissues over time; it can only slow them down (Rouy *et al.*, 2005). Defrosting causes irremediable dissolution of numerous cells. Thus we can see that analyses carried out as part of a counter investigation are on a sample which is not rigorously structurally identical to that used in the previous analyses. The results obtained may be altered, thus complicating comparisons between the two analytical series and the counter-investigation can be challenged on the basis of this observation if these results prove to be significantly different.

What can be done if an investigation is challenged? The examining magistrate being neither a toxicologist nor a chemist usually seeks the opinions of several experts as to the credence to be accorded to the various analyses carried out and the interpretations placed upon them. If the experts' opinions differ (which is likely to occur with at least two of them when a counter-investigation is required), the magistrate has three options: (1) disregard the toxicological evidence and concentrate on the other aspects of the case (fingerprints, witness statements, etc.), (2) go with the opinion of the most persuasive expert (the scientific criteria giving way in the end to more subjective criteria), (3) put his faith in the opinion put forward by the majority of the experts. In the latter case, we will see in section 5, which is dedicated to inter-laboratory tests, that placing trust in the largest number is an attitude that is open to debate from an epistemological point of view.

### **3. Problems Associated with the Absence of Standard Compounds**

As raised in paragraph 1.1, using an internal standard specimen for titrating molecules by GC-MS or LC-MS is essential. The function of the internal standard specimen is to reduce to a minimum the uncertainties concerning the result of the titration, but also to guarantee that the entire analytical protocol has taken place according to the validated procedure. To this end, the internal standard specimens must be added to the reference matrix when the test sample is taken and before it is prepared. Nowadays, whenever possible we use an analogue of the analyte marked

with stable isotopes ( $^{13}\text{C}$  or  $^2\text{H}$ ) as a standard specimen. For example, perdeuteronaphthalene constitutes an ideal standard for titrating naphthalene. There are two advantages of using a marked product. The marked analogue possesses ‘almost’ the same chemical properties as the analyte and will therefore behave in the same way as the analyte at all stages of sample preparation as well as during chromatography and mass spectrometry. Furthermore, the marked compounds are not naturally present in the environment. So using a non-endogenous molecule guarantees that the concentration of the standard is not distorted by its natural presence in the samples to be analysed.

Among the various problems posed by internal calibration, the difficulties relating to the absence of a suitable standard, to titrating very complex mixtures as well as those inherent in gas analysis are covered.

### 3.1. Difficulties Related to the Absence of a Suitable Standard

The absence of a suitable standard specimen is a problem frequently encountered when titrating polymers insofar as their synthesis is in general not totally mastered (Rial-Otero *et al.*, 2009). Polymers are generally made up of a mixture of a very large number of molecules of different sizes and in different proportions, each molecule being characterised by the number  $n$  of motifs (monomers) from which it is formed. Consequently, the chromatographic analysis of a polymer usually provides a chromatogram showing a very large number of peaks distributed over a wide range of retention times. Whatever the type of detector used, the response coefficients of the various components vary as a function of the length of the polymer chain. It is impossible to envisage titrating accurately each of the components in the mixture, which would require having all the components in a standard form, i.e. pure or in solution in a solvent at an accurately known concentration. It is not possible precisely because currently we do not know how to synthesise these molecules with total selectivity. Under these conditions, no titration can provide accurate results, the plot of a response function, even for external calibration (i.e. without an added standard specimen) is being totally compromised by the absence of a standard. Unable to do better, we limit ourselves more often than not to empirically estimating the overall quantity of polymer and indicating the relative proportions of the components, dividing them into families according to the number of monomers from which they are composed ( $1 < n < 10$ ,  $11 < n < 20$ ,  $21 < n < 50$ ,  $51 < n < 100$ ,  $101 < n$ , for example).

The analysis of Short Chain Chlorinated Paraffins (SCCP) ( $C_{10-13}$ ) in water constitutes a second relevant example. These compounds present as complex mixtures comprising several thousand positional isomers (Bayen *et al.*, 2006). So an SCCP chromatogram recorded by GC–MS using electron attachment ionisation shows a jumble of badly separated chromatographic peaks. The analysis is based on the integration of all the chromatographic peaks (sum of the areas). The concentration obtained is an average mass of all the molecules comprising the SCCPs. Clearly it is not possible to manufacture an analytical standard specimen along with its marked counterpart by complying scrupulously with the same composition as the commercial mixtures. SCCP standard specimens with variable percentages of chlorine are reconstituted from individual chloroalkanes in C10, C11, C12 and C13. They enable an overall estimate of the SCCP concentration to be made but in no way a titration of each.

### **3.2. Difficulties Relating to Calibration for the Titration of Complex Mixtures**

Two types of product perfectly illustrate the difficulty in titrating complex mixtures: essential oils and petroleum extracts.

Essential oils are very widely used in the food flavouring, perfume and cosmetic industries. Most of them are made up of dozens indeed hundreds of compounds in proportions varying from ppm (parts per million) to several dozen percent. Their analysis is therefore as awkward as the extremely varied chemical nature of the compounds present: terpenes, aldehydes, ketones, carboxylic acids, alcohols, amines, sulphurated compounds, etc. (Marriott *et al.*, 2001). So although the chromatogram of an essential oil is often very complex, that of a perfume made up of a mix of various essential oils and synthetic molecules can prove to be inextricable! An accurate quantification of the compounds present would involve not only using as many internal standard specimens as chemical families represented but also providing several response functions per molecule, the dynamic ranges supplied by the GC–MS and LC–MS devices not exceeding 500 to 1000 in the best case scenarios. For example the limonene molecule (allergen) is present in almost all essential oils. It constitutes up to 85% of an orange essential oil while its concentration does not exceed a few ppm in certain perfumes. A given response function would not therefore be able to titrate limonene in all types of flavouring or perfume. Several methods should therefore be available for titrating each of the compounds liable to be present in trace amounts or in abundance in the sample.

Moreover, given that the composition of an essential oil varies from harvest to harvest depending on the amount of sunlight, rainfall etc., and that this composition varies over time depending on transport and storage conditions; we cannot hope to obtain a ‘universal’ reference. All these reasons mean that it is almost impossible to envisage accurately titrating each component of a perfume. We generally have to content ourselves with approximate results.

In a radically different sector, the analysis of petroleum products presents the same kinds of difficulties. The fuels extracted from petroleum are indeed also made up of hundreds of molecules with different chemical structures (Blomberg *et al.*, 2012). Although hydrocarbons make up most of these, they also contain non-negligible proportions of oxygenated, nitrogenated and sulphurated compounds etc. It is almost impossible to separate all these constituents even using two-dimensional chromatography (Christensen & Tomasi, 2007). We can accurately titrate a family of compounds, but not each of the constituents of fuel for the reasons given above.

In principle, there is no reason why we couldn't consider titrating all of these molecules if we had unlimited time and financial resources. We could design a method in which the petroleum extract would be broken down initially into a very large number of samples by preparative chromatography. Each of these samples would then be analysed using GC–MS, LC–MS or both, after having synthesised and purified the dozens of standard specimens (unmarked molecules and molecules marked with stable isotopes) needed to build the various response functions. Note that it would be necessary to produce multiple response functions for certain components liable to be present in the fuel over a very large range of concentrations. The optimisation and validation of such a method would require months, perhaps several years of work. Each analysis would take several days and would represent an enormous financial cost. The examples above illustrate the fact that the limits of chemical analysis are not necessarily down to the knowledge and skills of the chemists. They are sometimes dictated by challenges not directly related to science.

### **3.3. Difficulties Relating to Calibration for the Analysis of Gases**

The analysis of gases remains a real analytical challenge even today. It most often uses so-called ‘head space’ techniques. When we want to titrate one or more volatile compounds on the surface of a liquid, we can use fibres like Tenax® or PDMS (PolyDiMethylSiloxane) for example to

capture them. The compounds we want are absorbed on the fibre according to their chemical affinity (in particular their polarity). The fibre is then introduced into the injector of a gas chromatograph where the heating desorbs the captured molecules. This technique, called 'SPME' for 'Solid-Phase Micro Extraction' is in widespread use. It has undergone significant improvements in recent years with the appearance of automatized apparatus for sample preparation that allow the temperature of the gas and liquid phases to be controlled in particular, and to vibrate the fibre so as to reduce the equilibration time between absorption and desorption of the molecules in the gas phase (Wang *et al.*, 2008). It has been established that adding a suitable internal sample specimen (compound marked with stable isotopes) for each of the molecules to be titrated in the liquid phase (standard sample which will divide itself between the gas phase and liquid phase according to its vapour pressure) allows relatively accurate titrations to be carried out on condition that we work with few analytes and over a small dynamic range for each.

The analysis becomes more awkward when we are no longer analysing a gas phase on the surface of a liquid in an enclosed space, but titrating volatile molecules in the atmosphere. In this case, the simplest sampling method is to let the atmosphere penetrate a container, stop it off then connect it to a mass spectrometer. The internal atmosphere in the recipient is then 'sucked' by the vacuum in the spectrometer. The disadvantage in this case is that the analytes will not be separated by chromatography. When the analytes are much diluted in the gas, we can diffuse the latter in a trap (absorbent surface or cryogenic trap) to concentrate the compounds before analysis by GC-MS. In all cases of atmospheric analysis, it is almost inconceivable to add an internal standard specimen into the atmosphere prior to capturing the desired molecules, which leaves the analyst with significant uncertainties as to the results of the titrations.

#### **4. Questions Related to the Applicability of the Method in Real Cases**

A major problem posed by the method described above is in the addition of standard molecules to the reference matrix exogenously. Let's consider the example of titrating pesticides in salad vegetables. Clearly, the physicochemical interactions between the pesticides and the matrix will not be the same depending on whether the pesticides have been added in solution then mixed with the chopped up salad sample or introduced via the roots and carried into the leaves by the sap. They will be considerably more difficult to extract in the second case. This is why the sample

preparation protocol developed on a doped reference matrix can turn out to be inefficient with real samples.

The case of a toxicological analysis such as the titration of LSD (lysergic acid diethylamide) and its metabolites in the blood is even more critical. During the development of the method, blood that is free of LSD is doped with LSD and metabolites at known concentrations to calibrate the method (Libong *et al.*, 2003). The sample preparation is optimised from these doped solutions. LSD present in real samples had been swallowed then had migrated quickly in the blood through the tissues, and had traversed various organs within which it had been metabolised. Naturally, the physicochemical interactions between LSD and the various components of the blood (plasma, red blood cells, platelets, etc.) circulating in an organism are totally different from those which take place when LSD is added to blood in a test tube. The last step in validating the method generally involves testing with real samples, i.e., we titrate LSD and its metabolites in the blood of an individual who we know has recently consumed this narcotic and check that we detect the molecule and its metabolites. Although detecting these is evidence of the effectiveness of the method, the concentrations measured are complete unverifiable, all the more so as metabolism varies between one individual and another.

The problem described in the above example becomes much more complicated still when transposed to a medico-legal or 'forensic' investigation. In the latter case, the chemical composition of the blood varies considerably from one victim to another as a function in particular of the time elapsed between the death and the discovery of the body and the state of preservation of the latter (temperature, immersion in water, etc.). The blood quickly becomes like lacquer (very viscous, indeed solidified) after death, and it is difficult to envisage from a technical point of view developing the sample preparation by doping the blood taken after death with the narcotic and its metabolites. Consequently, the analyses carried out in medico-legal toxicology use methods initially developed for clinical toxicology with processes for extracting compounds that are not really suitable for actual samples. It is generally accepted by the experts that this method of working, although not ideal, constitutes the least worst option available to us. Would it be better to have no toxicological investigation at all rather than one where the detected quantities come with a health warning?

## 5. Interpretation of Inter-laboratory Tests

Method validation is a quality procedure carried out internally within a laboratory or a company whose final step is to test the applicability of the method on actual samples with the above-mentioned difficulties. So with the objective of evaluating their performances and comparing them with partner or competing laboratories, certain laboratories take part in inter-laboratory test campaigns. The principle is very simple: several laboratories working in the same area (health inspection of foodstuffs for example) receive the same sample to analyse. The results are returned to the participating laboratories in the form of statistical data, anonymously, each laboratory being allocated a number. Figure 2 (below) shows an example of the distribution of results obtained by ten laboratories following the titration of two pesticides in the milk from a cow. These are fictional results intended to illustrate our argument, the data for this type of test generally being sent exclusively to the laboratories involved.

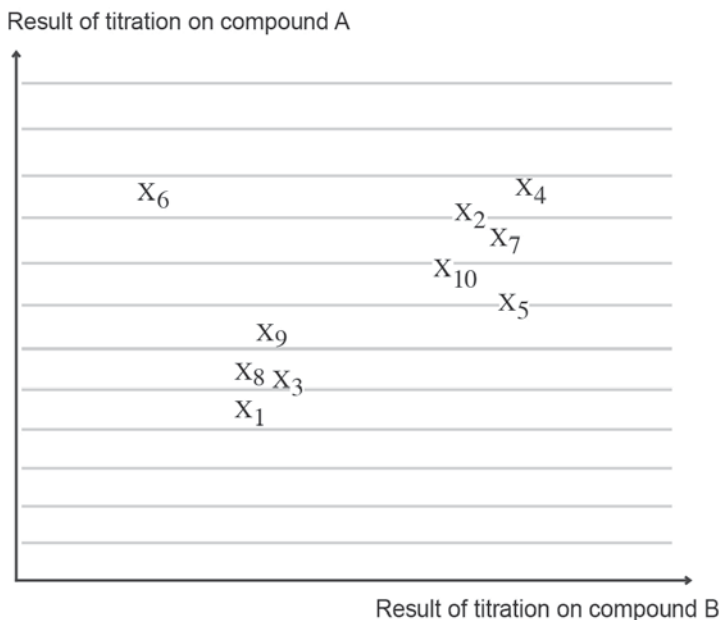


Figure 2. Presentation of the results obtained by 10 laboratories following the titration of two pesticides labelled A and B in the same sample of cow's milk.



Figure 2 shows that laboratories 2, 4, 5, 7 and 10 obtained values close to one another at the end of the two titrations. The four laboratories 1, 3, 8 and 9 provided values very close to one another but relatively far from those from laboratories 2, 4, 5, 7 and 10. As to laboratory 6, the results obtained departed from the others in figure 2, with in particular, a value for the concentration for component B significantly less than those measured by the nine other laboratories.

Inter-laboratory tests frequently lead to results dispersed in this way. How may we interpret figure 2? There is no clear answer to this question. Some would consider that laboratories 2, 4, 5, 7 and 10 are the most efficient as they are among the greatest number to supply analogous results. To say that the greatest number must be correct is to effectively apply democratic political principles to science. In this example, this option would seem very debatable, particularly as laboratories 1, 3, 8 and 9 also gave results that agreed and were consistent with each other. To consider that the laboratories which measured the highest value of A are the nearest to the actual figure because there were 5 of them while 'only' 4 provided a lower figure would appear to be a simplistic way of assessing the relative performances of the various laboratories. As to the chemists in laboratory 6 whose results did not agree with any of the other nine laboratories, some would consider that they should change their analytical methodologies, others that they were the only ones to come close to the real situation, like Galileo in his time! Although democracy often appears as the 'least worst political system' (to paraphrase Winston Churchill), there have been many examples in history where it has given power to individuals with very questionable morals! Statistics, a very powerful research tool in a number of areas, can sometimes appear as a method of last resort in the analytical sciences with regard to giving confidence as to the relevance of the results obtained when many sources of uncertainty remain. In the example above, it would be possible to carry out statistical calculations on the variables to produce means and standard deviations, but the statistical result does not answer two crucial questions posed by the results of this study: Who gave the 'correct' result (if the 'accurate' result had indeed been found)? Why is there such a discrepancy in the measurements? We could always increase the number of laboratories taking part in the tests using the currently accepted postulate that the higher the number of experimental results the more accurate the statistics will be, but we will never be able to answer the above questions using mathematics.

If we accept that no one knows the 'true' result, i.e. the actual concentrations of analytes in the matrix as mathematically defined in the international chemistry baseline ( $C=n/V$  where  $C$  is the concentration,  $n$

the quantity of material and  $V$  the volume of the matrix), the solution which readily springs to mind as the most rational is to say the result produced by the greatest number is correct over the one laboratory which produced results widely differing from those of the other laboratories. Although this may be a legitimate postulate in a basic mathematical model (result repeated and near to the arithmetic mean), it is much less so from epistemological point of view. Indeed, to consider that the average of the five closest results to be the 'accurate' result comes down to saying that these laboratories have produced, not a value which relates to 'reality', to 'what really exists', but a reference value for the scientific community. It would only take one of these laboratories to find a different result (or not take part in the study) for this reference value to be changed. We are therefore forced to admit that not only does the baseline according to which we study the reproducibility of the analysis change according to the results obtained from those taking part in the research but also that each does not contribute equally to this change, in particular if we discard results considered as erroneous on the basis of scientific calculations.

To conclude, it is absolutely not a question of denying the relevance of carrying out inter-laboratory tests. To compare results and encourage exchanges and discussions on the methodologies can only be extremely beneficial to the scientific community as well as for those who request analyses (the medical world, industrial companies, public authorities, etc.). We can only encourage these types of test. However, we must remain cautious as to the statistical inferences we draw from the results. Indeed, although values such as an average, variance or standard deviation may be highly relevant to, as an example, establishing the reproducibility or robustness of a method, they can only be used in the mathematical baseline defined for the relevant calculations. They can in no way constitute a way of describing the actual situation as defined above.

This example illustrates the tendency amongst chemists to invent ways of assessing and studying singularities. They do not think in terms of generalities and generalisations but rather reason pragmatically and continually invent models adapted to the singularities. This observation, specific to the activity of chemists, demonstrates the necessity of having a philosophical discussion on these modelling and analytical practices.

## 6. Limits of Environmental Standards

Chemical analysis is often carried out within the scope of national or international standards. A standard is defined as follows: 'a document, established by consensus and approved by a recognized body, that provides,

for common and repeated use, rules, guidelines or characteristics for activities or their results, aimed at the achievement of the optimum degree of order in a given context<sup>1</sup>. We will consider here those environmental standards currently of concern, which occur repeatedly at the heart of a number of political debates. The European Parliament's 'REACH' directive (Registration, evaluation and authorisation of chemicals), covered very prominently in the media, is a particular case in point in this context as it is based essentially on an assessment of the toxicity and full market approval of chemical substances<sup>2</sup> (25). Most environmental standards lay down, for one or more given classes of molecules, maximum concentrations that must not be exceeded in a given matrix. They could, for example, give maximum admissible concentrations of nitrates and pesticides (among others) for which water could be declared fit for drinking, maximum hydrocarbon levels for seawater and neighbouring beaches to be considered 'unpolluted' following an oil spill. As far as toxicology experts are concerned, a concentration has to be set for each substance or family of substances beyond which the matrix is judged to be unfit for consumption (drinking water, various foodstuffs), or unsuitable for tourists (bathing waters, beach sand, etc.) for example. Establishing this value can clearly be open to criticism as it is complex: not only do toxicity levels vary from one individual to another depending on criteria such as age, sex or body weight, but the attendant presence of multiple toxins and/or certain molecules making up the matrix can induce agonist or antagonist effects on the overall toxicity of the mixture. The chemists do not ask themselves about the relevance of this value but the detection limit of their titration method for a forbidden substance (tolerance zero) or the accuracy of their method around this value for a so-called 'threshold' substance. The intention of this section is not to list once again the numerous difficulties inherent in titrating analytes in a matrix stated previously, but to question the decision-making process following the analysis in this context. As we have seen, an analytical method, even one validated according to drastic criteria, provides results which have a degree of uncertainty. We must therefore take this uncertainty into account when we compare the result found with the value laid down by the standard. The problem is that this uncertainty cannot always be quantified. Although it is easy to estimate the uncertainty associated with the use of a classical measuring instrument (pipette, weighing machine, pH meter, etc.), it is not possible to precisely quantify the error introduced due to

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<sup>1</sup> Please refer to 'Directives ISO/CEI. (2004). Partie 2: Règles de structure et de rédaction des Normes internationales, cinquième édition, (Chapitre 3.1.)'.

<sup>2</sup> Please refer to 'Règlement (CE) n° 1907/2006 du 18 décembre 2006 (REACH)'.

validating a method from a *model* (a matrix with questionable representativeness doped with analytes) and then applying it to real environmental samples. How, under these conditions, can the area of reliability of this method be defined? By extension, how can we decide whether a result slightly below the decision threshold value can potentially translate into a 'true' value greater than this reference value when the difference between the result found and the decision threshold value is small in comparison with the measurement uncertainties. The concept of the precautionary principle, already contained in the procedure used to set a decision threshold value suggests taking into consideration a wide interval of uncertainty around the value measured before comparing it with the reference value. The question remains to know how wide an interval is. How do we quantify it, when errors based on a change of baseline between the development and validation phases of the analytical process and the routine analysis on the actual sample are not quantifiable, precisely because this can only be done within a given baseline?

The standards in force have a technical, administrative and political use, but this example clearly illustrates the need to research into solutions to stabilise the results in a given research project. How can we invent a set of practices in order to evaluate, study and quantify singularities? We chemists are waiting for the philosophers to help us consider our relationship with the real world, to define the sciences and with the laws of measurements and models. This relates in particular to answering the following questions: what do uncertainties do? How do we make sense of measurements and on what are they based?

## Conclusion

The few examples presented above illustrate that, contrary to an idea currently widespread amongst the public at large, analytical chemistry is not based on incontestable truths but is the result of mutually stabilised scientific practices which aim to find a consensus on the quantification of singularities with all the difficulties this implies. Contrary to another widely accepted idea, the limits of this discipline are not only those imposed by the measuring instruments in terms of detection limits, accuracy and precision, for example. In many areas of analysis, the limits are set by the methodology itself and the definition of models, in particular by the absence of a relevant standard specimen or suitable reference matrix. In this context, we should put the technological path towards ever-lower detection limits using ever more costly equipment, a path that has a depressing effect on the least financially endowed laboratories. This is

clearly not to condemn technological progress, which has revolutionised analytical chemistry over the last century and continues with no doubt to improve its performance at a spectacular rate. Rather when carrying out analytical developments, we should be asking ourselves about the suitability of the precision provided by the measuring instruments relative to the uncertainties inherent in the methodology chosen together with the implementation of consensus around the methods used. On the last point, the contribution of sociologists and philosophers could prove to be highly relevant. We should also be encouraging chemists not only to produce estimates of the uncertainties attached to the results wherever possible (which is still far from systematic today), but also to better inform their interlocutors (industrial companies, consumer associations, examining magistrates, politicians, etc.) as to the limits of the analytical methods with regard to the baselines used.

Analytical chemistry is above all a tool, a discipline in the service of numerous other sciences. In the vast majority of cases, the methodological limits described above are not too much of a problem as they are compatible with the current state of knowledge and allow us to give meaning to the comparisons on which environmental standards are based. Let's consider for example a burning topic currently in the news such as the contamination of river waters by endocrine disruptors. The question for our society relates to their toxicity with regard to the living organisms consuming these waters. Now we could legitimately consider that the above mentioned analytical uncertainties are low in proportion to the toxicity of the compounds we are interested in. Toxicology comes up against the same sorts of limits as analytical chemistry when, for example, it extrapolates toxicity values established in rats or rabbits to man. The question here is not about judging the relevance of this extrapolation, but about considering that the uncertainties to which it is subject are certainly much greater than those inherent in the analytical procedure. Consequently, the titration of endocrine disruptors provides information that is highly relevant to toxicology even if the methodologies available today are such that the results assume a high degree of uncertainty. If philosophers and historians were to carry out epistemological surveys on extrapolation practices currently in use by chemists, the results would be useful.

It is the role of everyone who implements methodologies and carries out analyses on a routine basis to continually ask themselves the relevance of the results provided and the interpretation which can be put on them. Although the methods are subject to criticism and not free of approximations in the examples presented above, they are not the less

legitimate for that in the contexts in which they are used as they make the analytical results intelligible and allow decisions to be taken. From a pragmatic point of view, it is clear that such methods have enabled considerable advances to be made in a number of areas (environment, public health, industry, etc.), advances which continue today in parallel with discussions which aim to improve these methods. In this regard we can only bemoan the fact that these discussions most often only take place between small numbers of chemical analysis specialists. Although the skills of the latter are undeniable, discussions between experts in the same scientific area generally lead to research into technical solutions or statistical calculations which are continually improving but which only touch on the uses to which they are currently put. This is why it would be highly desirable to invite science historians and philosophers to join in with these debates to allow us to take advantage of their detachment and instigate new discussions on certain contemporary chemical practices.

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# INTERDISCIPLINARY ISSUES IN NANOSCALE RESEARCH

JOACHIM SCHUMMER

## Introduction

Nanoscale research is currently attracting tremendous attention from both the general public (Schummer 2005) and from a large variety of science and engineering disciplines (Schummer 2004).<sup>1</sup> The attraction is largely fostered by technological visions, the promises of new scientific discoveries, and huge governmental funds. Such a melting pot of various disciplines promises to be a great opportunity for innovative research through synergetic effects, provided that researchers from different disciplines find a common basis required for interdisciplinary research. If that is missing, however, disintegration is to be expected and researchers will at best do their disciplinary research business as usual, though under a new label. Therefore, the understanding and mediating of interdisciplinarity is a crucial factor in the future success of nanoscale research. Yet, although every report on nanoscale research highlights the necessity of interdisciplinarity,<sup>2</sup> little effort at understanding interdisciplinarity has been made. To the contrary, there is currently a naive rush from badly understood interdisciplinarity towards new visions of super-interdisciplinarity to be centered on nanotechnology (Roco & Bainbridge 2002).

A sort of longish introduction, the first part of this paper presents some general ideas about interdisciplinarity and its related concepts, such as discipline, multi- and transdisciplinary, or super-interdisciplinary. The second part starts with a summary of scientometric findings about multi- and interdisciplinarity in current nanoscale research (Schummer 2004). Since these findings suggest that interdisciplinary nanoscale research is

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<sup>1</sup> This paper was first published in Davis Baird, Alfred Nordmann & Joachim Schummer (eds.), *Discovering the Nanoscale*, Amsterdam: IOS Press, 2004, pp. 9-20; reproduced with permission from the author.

<sup>2</sup> For a report that calls for interdisciplinarity even in its title, see Malsch 1997.

indeed in a bad shape, the rest of the paper analyzes two specific reasons for this. On the one hand, I argue that current definitions of nanoscale research, which are mainly based on the size of objects, are too vague to provide any integrative function. On the other hand, I point out that certain discipline-rooted technological paradigms, such as “self-assembly” and “atom-by-atom-manipulation”, which are currently employed in nanotechnological visions, are barriers to interdisciplinarity insofar as they include metaphysical oppositions that disintegrate rather than integrate the disciplines.

## 1. Elements of Interdisciplinarity

### 1.1. A Brief Survey of the Literature

Strangely enough, the literature on interdisciplinarity is multidisciplinary rather than interdisciplinary (for the distinction, see below). It includes scholars from science education, sociology of science, history of science, and philosophy of science.<sup>3</sup>

As we shall see, the term “discipline” has strong educational connotations. A great part of the literature on interdisciplinarity therefore belongs to professional education and arose from debates about reforms of tertiary education to be based on a broadened scope of general knowledge, like a *studium generale*.<sup>4</sup> Other literature stems from sociology of science and science policy studies. Not surprisingly, scholars in these fields focus on sociological and organizational aspect of interdisciplinarity while neglecting to some extent the cognitive side. Much more integrative perspectives can be found in the numerous detailed case studies of interdisciplinary research and discipline formation by historians of science.<sup>5</sup>

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<sup>3</sup> Still the best survey with extensive bibliography is Klein Thompson 1990; a more recent bibliography has been prepared by Brandl 1996. Recent monographs and anthologies include Kline 1995, Klein Thompson 1996, Galison & Stump 1996, Umstätter & Wessel 1999, Weingart & Stehr 2000, Käbisch, Maaß & Schmidt 2001, Moran 2002; see also the ongoing online discussion of papers published since April 2003 by Interdisciplines [<http://www.interdisciplines.org/interdisciplinarity>].

<sup>4</sup> A great many books with “interdisciplinary” in their titles result from *studium generale* lecture series on some topic with speakers from different disciplines. All of these books that I have seen are really multidisciplinary, that is, a collection of disciplinary essays without any reference to each other.

<sup>5</sup> For nanoscale research the most relevant recent case study is on the discipline formation of materials science since about 1960, see Bensaude-Vincent 2001.

When sociology and history of science merge, this frequently results in “Big Philosophical Pictures”. A favorite topic is the allegedly new or hoped-for interdisciplinarity between science and technology in problem-based research, for which historical claims have been made and new terms introduced, like “Technoscience” and “Mode 2 of Knowledge Production”. Such approaches may belong to philosophy insofar as they engage in metaphysical and epistemological debates about modernism and post-modernism or realism/constructivism rather than the historiography of science. In fact, they, more or less explicitly, oppose the other Big Philosophy Picture of interdisciplinarity, the ambitious Unity of Science Project launched by Logical Positivists in the 1930s. Claiming that the disciplinary languages of all sciences can and should be based on or reduced to the language of physics, the Unity project reduced interdisciplinary relations to the reduction of all sciences to physics. With their bias towards physics, modern philosophers of science (or rather, of physics) favored physicalistic reductionism as the only interdisciplinarity relation, be it on the level of descriptive language, theories, so-called meta-theories, ontologies, or methods.<sup>6</sup>

It might be recalled, however, that the cognitive relations between the sciences, or more generally the structure of our overall knowledge, has been a central topic of philosophy ever since at least Aristotle. Behind this stands the classical idea that the ideal structure of our knowledge does or should correspond to the structure of our world—a position that has frequently recurred as either epistemological realism or metaphysical idealism. By emphasizing the impact of social dynamics on the structure of our knowledge, social constructivists could easily challenge the classical idea, particularly in its epistemological version, with case studies on the social dynamics of the disciplinary structure, provided that the disciplinary structure determines the structure of knowledge. This has made interdisciplinarity a hot topic, although full of ambiguity as to whether “discipline” is considered a cognitive or a social category and as to whether epistemological claims are meant to be descriptive or normative.

## 1.2. What is a Discipline?

In its original Latin meaning, which is still preserved in current English as well as in other European languages, the term “discipline” (from Latin, *disciplina*) refers to a body of knowledge that is taught in a certain school. Students (disciples) learn a certain doctrine (a discipline) by obeying strict

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<sup>6</sup> For an excellent account of the manifold “fallacies of projection” from physics to other discipline, see Kline 1995, particularly part 4.

(disciplinary) rules of a school (discipline) and by practicing self-control (discipline). There is no disciplinary knowledge without a social context of transmission and education and a social body that thereby reproduces itself. Modern scientific disciplines do not differ much from that, except that they do not simply preserve but increase and modify a body of knowledge through scientific research—which requires even stricter methodological rules to preserve the continuity of the social body. Thus, a scientific discipline, as I will use the term in the following, comprises both cognitive and social aspects: (1) a body of knowledge, including concepts and beliefs (knowledge of objects), methods for increasing and securing knowledge (knowledge of methods), and values about judging the quality and importance of knowledge (knowledge of values); (2) a social body with effective rules and means for increasing, communicating, and teaching the body of knowledge as a way of self-reproduction.

### **1.3. Multi-, inter-, Transdisciplinary, and Superinterdisciplinary**

The terms “multidisciplinary”, “interdisciplinary”, and “transdisciplinary” have been used to describe research activities, research problems, research institutions, teaching, or a body of knowledge, each with an input from at least two scientific disciplines. Although confusion still abounds, there is some agreement that “multidisciplinary” describes a rather loose, additive, or preliminary relation between the disciplines involved, whereas “interdisciplinary” requires stronger ties, overlap, or integration. In some diachronic models, multidisciplinary is a preliminary step toward interdisciplinarity, which can go as far as to either unify two or more disciplines or to create a new “interdisciplinary” (hybrid) discipline at the interface of the mother disciplines. “Transdisciplinarity” is a diachronic (if not a political or “antidisciplinary”) concept to describe a state of research or knowledge that transcends disciplinary boundaries, with continuous input from various disciplines but without any inclination to consolidate into a new (hybrid) discipline. On the opposite side of this is “superinterdisciplinarity”, a term used to describe a new unity of all or at least of many sciences.

### **1.4. Cognitive Elements and Strategies of Interdisciplinarity**

Cognitive elements of interdisciplinarity follow from our definition of a discipline. People from different disciplines involved in a common interdisciplinary research project must share a common knowledge basis, con-

sisting of knowledge of objects, methods, and values. As long as there are different disciplines in the proper sense, the common basis can only consist in more or less overlap, because disciplines greatly differ in their knowledge of objects, in their methods for increasing and securing knowledge, and in their values about judging the quality and importance of pieces of knowledge. There are three approaches to increase overlap.

- (1) *Reductionism* tends to ignore the differences of knowledge bodies by inventing hierarchies, such that the knowledge on one level can be reduced to the knowledge on a more basic level. The price of reductionism, which has been favored by many philosophers of science (of physics), is that their picture of scientific knowledge has lost any descriptive value with regard to the actual sciences other than physics.
- (2) *Simplification* is a strategy that largely relies on the common ground of everyday knowledge. Because we share to some extent a common experience, an ordinary language, a rich source of common metaphors and pictures, this is a useful point to start with. Since ordinary knowledge does not capture the sophisticated structures of disciplinary knowledge, crude over-simplifications and particular efforts at using visual forms of communication are typical approaches that are all too apparent in current nanotechnology. The risk of simplification is that people stick to artificial problems and solutions, created from oversimplification, and that they do not recognize that simplification can only be a preliminary step towards serious research.
- (3) *Translation or Mediation* requires a translator who should ideally be educated in all the disciplines involved. This would certainly be the best solution if mediators were available and socially accepted, neither of which is the case. Alternatively, scientific education could provide a broad scope of multidisciplinary teaching to students, such that everybody involved in interdisciplinary research has at least a basic understanding of the other disciplines. However, the general trend of tertiary education is heading in the opposite direction, which leads us to social elements of interdisciplinarity.

### 1.5. Social Elements of Interdisciplinarity

Long before the formation of a new discipline comes the step from multi- to true interdisciplinarity. It requires a considerable effort of social integration that involves new infrastructures for communication, collabo-

rative research, publication, and teaching. While these aspects have been dealt with at length in the sociology and science policy literature, I would like to point out two further interrelated factors of social integration that are frequently overlooked because they appear to be only about cognitive integration. Both play a growing role in current nanoscale research, they are the historiography of the field, and its visions. As they look into the past and into the future, both frequently appear in the same sort of texts authored by leaders in the field, namely in introductory, review, and editorial essays.

By identifying the founders and heroes of a field, both the field and the community are shaped, if not created.<sup>7</sup> In addition, references to early and widely accepted authorities add seriousness and attractiveness to the field. A powerful tool of discipline formation, self-historiography frequently appears at the earliest state when research is just at the beginning. Two famous historical examples are Priestley's history of electricity from as early as 1767 and Ostwald's history of electrochemistry from 1896. Moreover, historiography takes a dynamic view of the field. It first places current activities into the overall historical development, and thereby provides historical meaning, significance, and links to the current works of researchers. Secondly, it calls for, or is even recruited for, extrapolation to the future, thereby giving plausibility to visions as the natural outcome of the historical development. That is why historiography and the formulation of visions frequently appear closely together.

Visions add further meaning, orientation, and links to particular research projects. Expressed in simple terms with reference to general human needs, visions provide quick answers to why-questions of a general audience—questions which researchers in highly specialized fields have difficulties to answer otherwise. By sharing the same visions, researchers of different fields can see each other as working on the same project or even belonging to the same community. This is the positive aspect of the current production of nanotech visions. Later we will see that visions can also pose barriers to interdisciplinarity.

## **2. The Basis of Interdisciplinarity in Current Nanoscale Research**

In this section, I first present some scientometric results about the disciplinary structure of current nanoscale research and then discuss two elements on which expectations of successful interdisciplinary research

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<sup>7</sup> For a case study on the historiography of psychology, see Geuter 1983.

largely seem to be based: the length scale of objects and technological visions about future success. The idea behind that seems to be straightforward: in order to integrate a bunch of scientific and engineering disciplines into one project, they must first study the same objects and secondly have the same vision of what the research should aim at technologically—interdisciplinary collaboration will then follow automatically. We will see that this is not that easy.

## 2.1. Multidisciplinarity and Interdisciplinarity in Nanoscale Research Journals

The journals in which nanoscale research is published are a good source to analyze its multi- and interdisciplinary structure. Although much of nanoscale research is still published in classical disciplinary journals, there are already eight journals devoted to the new field.<sup>8</sup> In the following, I will focus on two journals: *Nanotechnology*, published since 1990 by the UK based Institute of Physics, with 150 regular papers in 2002; and *Nano Letters*, published since 2001 by the American Chemical Society, with 281 papers in 2002. Both journals define their field quite similarly as nanoscience and nanotechnology, and both have an explicit interdisciplinary mission ventilated in their Aims-and-Scope sections.

If one looks at the disciplinary affiliation of the authors, as I have done with 100 papers of each journal (see Figure 1), the combined results present a rich spectrum of all the disciplines involved in nanoscale research, i.e., physics, chemistry, materials sciences, electrical engineering, chemical engineering, and so on. In contrast, in a typical disciplinary journal, e.g. the *Journal of the American Chemical Society* (JACS), about 80% of the authors are from the “mother discipline”, with some 20% from neighboring disciplines. From that we may conclude that nanoscale research is in fact multidisciplinary.

Yet, the disciplinary landscape becomes more divided when we analyze each of the two journals separately (see Figure 2). It turns out that we have a “nanophysics” journal with almost half of the authors from physics; and a “nanochemistry” journal with almost half of the authors from chemistry. Also, both journals show some preferences for favorite “guest disciplines”—particularly the physics journal for electrical engineering and chemistry, and the chemistry journal for physics and materials sciences.

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<sup>8</sup> The results of this section are taken from a much more comprehensive scientometric study of eight nano journals, which also includes details on various methods of measuring interdisciplinarity (Schummer 2004).

Still, the overall picture of each journal is more multidisciplinary than disciplinary journals like JACS.

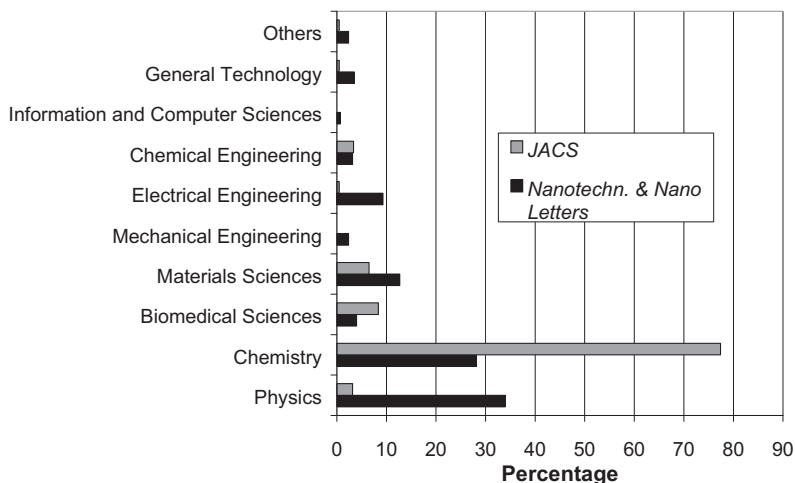


Figure 1. Disciplinary affiliation of authors publishing in “nano journals” (*Nanotechnology* and *Nano Letters*) as opposed to the disciplinary *Journal of the American Chemical Society* (JACS) (data from Schummer 2004).

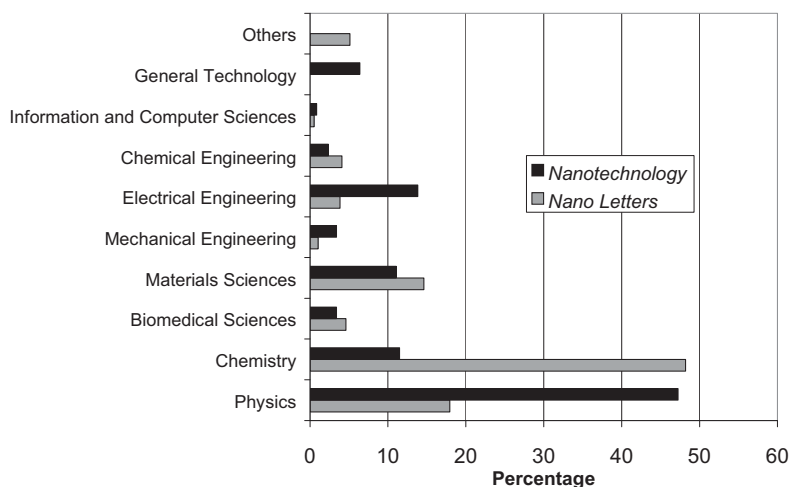


Figure 2. Disciplinary affiliation of authors publishing in *Nanotechnology* and in *Nano Letters* (data from Schummer 2004).



However, a multidisciplinary journal does not necessarily contain interdisciplinary research, since each discipline could publish its papers separately. Interdisciplinary research requires that scholars from different disciplines collaborate to become co-authors of one paper. On average, a paper in nanoscale research has 4.5 authors from 2-3 different institutions; in this regard, it does not much differ from a typical disciplinary journal like JACS. The question is if the different institutions belong to different disciplines, instead of being located just in different cities. A simple measure for interdisciplinarity of a journal is the number of papers with authors from more than one discipline, the *interdisciplinarity rate* (see Table 1). The surprising result here is that our nanoscale research journals, though being more multidisciplinary, are hardly more interdisciplinary than a typical disciplinary journal like JACS.

**Table 1: Interdisciplinarity rates and main bi-disciplinary Collaboration**

Journals	Interdisciplinarity rate (%)	Main bi-disciplinary collaboration
<i>Nanotechnology</i>	37	Physics & Chemistry (6%)
<i>Nano Letters</i>	37	Chemistry & Physics (12%)
<i>JACS</i>	30	Chemistry & Materials Science (9%) Chemistry & Biomedical Sciences (9%)

I will now discuss two possible reasons why multidisciplinary of nanoscale research does not automatically lead towards interdisciplinarity.

## 2.2. The scale of objects as a common basis

Definitions of nanoscale research define this field almost tautologically by the nanometer size of its objects. For instance, the US committee on Nanoscale Science, Engineering and Technology (NSET) defines nanotechnology as:<sup>9</sup>

Research and technology development at the atomic, molecular or macromolecular levels, in the length scale of approximately 1-100 nanometer range, to provide a fundamental understanding of phenomena and materials at the nanoscale and to create and use structures, devices and systems that

<sup>9</sup> NSET, February 2000:

<[http://www.nsf.gov/home/crssprgm/nano/omb\\_nifty50.htm](http://www.nsf.gov/home/crssprgm/nano/omb_nifty50.htm)>

have novel properties and functions because of their small and/or intermediate size.

Since that is a precise length range, one might think that the definition of research objects is sufficiently clear. However, while it clearly defines a field of optical research, i.e. electromagnetic waves from far UV to soft X-ray, it is difficult to find any kind of matter that would not qualify as an object of such nanoscale research. The only candidates that come to mind are the small molecules and simple ideal crystals that fill introductory textbooks of chemistry—but even those have critical nanometer lengths in the gas phase at appropriate pressures, for example the mean free path length. Nowadays chemists produce more than fifteen million new substances per year, of which virtually all have molecular or crystallographic lengths larger than 1 nm.<sup>10</sup>

**Table 2: Examples of commonly known substances with crystallographic lengths in the nanometer scale**  
(data from <http://www.reciprocalnet.org>)

Substance Name	Empirical Formula	biggest crystallographic unit cell length
Formic acid	CH <sub>2</sub> O <sub>2</sub>	1.02410 nm
Buckminsterfullerene	C <sub>60</sub>	1.40410 nm
Glucose	C <sub>6</sub> H <sub>12</sub> O <sub>6</sub>	1.48400 nm
Gypsum	H <sub>4</sub> CaO <sub>6</sub> S	1.52010 nm
Vitamin C	C <sub>6</sub> H <sub>8</sub> O <sub>6</sub>	1.71000 nm
Alanine	C <sub>3</sub> H <sub>8</sub> ClNO <sub>2</sub>	1.75900 nm
Sulfur	S <sub>8</sub>	2.43360 nm
Vanillin	C <sub>8</sub> H <sub>8</sub> O <sub>3</sub>	2.50990 nm
Cholesterol	C <sub>27</sub> H <sub>46</sub> O <sub>1</sub>	3.42090 nm
Vitamin D3	C <sub>27</sub> H <sub>44</sub> O	3.57160 nm
Pepsin		29.01000 nm

Against the rhetoric of novelty, Table 2 provides a few examples of commonly known substances with crystallographic lengths in the 1-30 nm range. The celebrated “nano-substance” buckminsterfullerene is only slightly bigger than the simplest organic acid, formic acid, and smaller than everyday substances like sugar (glucose), gypsum, or vitamin C, which has long been produced at large industrial scale. Even elements,

<sup>10</sup> More exactly, Chemical Abstracts registered 15,459,282 new substances in 2003 of which 13,808,462 were biosequences (CAS 2004, p. 7).

such as sulfur, arsenic, antimony, and bismuth, crystallize with characteristic lengths in the nanometer scale. Typical substances of 20th-century organic chemistry, here exemplified by the flavor vanillin, the steroid cholesterol, and vitamin D3, are in the range of 2-4 nm. Depending on the number and constitution of their “building blocks”, amino acids, proteins cover a large range of lengths. Simple amino acids, such as alanine, already crystallize with lengths in the 1-2 nm range. The small-to-medium-sized protein pepsin, first isolated by Theodor Schwann in 1836, is almost 30 nm large.

Besides chemistry, almost every other branch of the experimental sciences and technologies deals with material objects structured at the nanoscale. Since it applies ubiquitously, the nanometer scale is insufficient to define any particular or new kind of research.

There is a popular view of the sciences, according to which a hierarchy of material objects is mirrored by a hierarchy of the disciplines: the basic science (called physics) deals with the “smallest” objects, elementary particles or atoms, that are the building blocks of the objects of the next level, namely molecules which define the field of chemistry. Next comes biology that deals with living beings that are made up of molecules, and finally, if you wish, sociology. Not surprisingly, that originally pre-modern view found expression in the 19th century, when the rapid formation and differentiation of scientific disciplines broke up old dreams of the unity of science. No doubt, creating a new unity of the sciences by conceiving a division of labor according to the scale of their objects served as a sedative for those who wished to hold on to such unity. However, this never had the slightest basis in the actual practice of the sciences. All of our sciences deal or could deal with objects of all length scales, ranging at least from picometers to meters. All combine various micro- and macro-perspectives, and sometimes, as in bulk properties of substances, the size of objects does not even matter.

Regarding the issue of interdisciplinarity, the good news is that, unlike the pre-modern view of science, different disciplines can and do share research objects of the same size—indeed almost every interdisciplinary research is based on sharing the same objects. The bad news is, however, that the lengths scale of objects has never been the main criterion to define a research field; that the nanometer scale is anything else than new, as the phrase “intermediate size” suggests; and that a shared scale of objects is hardly sufficient to integrate different disciplinary perspectives.

Give a macroscopic object, say an old coin, for professional investigation to a chemist, an economist, and a historian, and you will hardly notice that they speak about the same object. This is even worse with objects

beyond human perception, because here our common ordinary life practices of characterizing and referring to objects fail. In the molecular world, we need sophisticated instruments for characterization. And instead of pointing to an object of common reference, it is symbolic, theory-derived representations to which we must at first refer in scientific communication. If a chemist, a biologist, and a physicist talk about a certain kind of molecule, they may have some idea of sharing a common object because they have shared some basic education at school. Yet, as professionals, each has a different understanding of what a molecule is and what its essential features are. The chemist might analyze the molecule in terms of functional groups or reactivity sites, the biologist might be looking for biological information or biological functionality, whereas the physicists could be interested in spatial structure or electromagnetic properties.

One need not be a constructivist to accept that the scientific objects of different disciplines considerably differ from each other because each discipline has another cognitive, instrumental, and problem perspective on objects. As a realist one can claim that all perspectives can be focused on the same “bare object”—yet what matters in science are not “bare objects”, nor the notorious “Building Blocks of Everything”, but scientific objects that considerably differ from discipline to discipline.

One might object that I have stuck to conventional science and ignored the important new features that appear at the so-called “threshold” of the nanoscale and which deserve to create a new research field on its own. After all, by varying the size of material objects at the nanoscale, we can tune many properties that depend on the electronic structure at the objects’ surface, like electromagnetic or catalytic properties. And by furthering supramolecular chemistry or by modifying the basic systems of genetic engineering, we could create new machine-like devices with new functionalities. That is all true, and promising indeed. However, just as the understanding of what a molecule is differs considerably between chemists, biologists, and physicists, so does their understanding of what a larger nanoscale object is. The size of objects simply does not matter. It is their disciplinary perspective that renders their objects different from or similar to each other, as a chemical reaction site or reactor, as a mechanical or electrical device, as a self-reproducing or information transmitting entity, and so on. In short, the idea that the common size of research objects might be a sufficient ground for the integration of various disciplines is misleading.

### 2.3. Technological Paradigms Underlying Nanotech Visions

Most reports about the prospects of nanoscale research refer to such values as health, wealth, security, and “environment”. These are so general that almost everybody would subscribe to them, regardless of their disciplinary professions. Through their appeal to general values or basic human needs, technological visions can provide some integration of different disciplinary perspectives. Yet, once the visionary ways by which such basic values could or should be realized technologically are spelled out, disciplinary distinctions appear. Scholars from different disciplines rely on different “technological paradigms”. On a very general level, a technological paradigm determines the scope of what is considered technologically feasible and how to approach a technological problem. Technological paradigms usually rest on past successful approaches within the discipline; they are applied to new issues by analogical or metaphorical reasoning rather than by deduction or scientific prediction; and they incorporate metaphysical concepts such as nature or the human-nature relationship.

Current prospects and visions of nanotechnology refer to several different technological paradigms, of which for reasons of brevity I discuss only the two most frequently mentioned: “atom-by-atom-manipulation” and “self-assembly” or “self-organization”.

*“Atom-by-atom-manipulation”* was fostered when scanning probe microscopes (STM, AFM, etc.) turned from mere surface imaging instruments (since about 1981) into surface imaging *and* “manipulation” instruments (since 1986), such that individual atoms could be moved and monitored almost simultaneously. Extending the approach to three dimensions, visionaries like E. Drexler conceived atom-by-atom-manipulation as the making of any molecular structure from individual atoms by sticking them together with ultra-atomic precision, once a suitable device—a so-called “universal assembler”<sup>11</sup>—has been manufactured. The technological paradigm behind this vision of a new way of doing synthetic chemistry is clearly derived from mechanical engineering by extrapolating high-precision manufacturing to the subatomic scale. (Correspondingly, Drexler’s vision of “self-assemblers” repeats the historical step from the manufacturing of machines to that of tool making machines.) Indeed, the most advanced approach in this field, namely micro-lithography, is also called the “top-down approach” of nanotechnology. “Atom-by-atom-manipulation” promises nanotechnological success by keeping to mechanical engineer-

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<sup>11</sup> Drexler (1986, chapter 1). Unlike Drexler, Stephenson (1995) used the term “matter compiler” which refers to computer science rather than to mechanical engineering.

ing's virtues of high-precision and complete human control over the technological process and also over the matter involved, to the extent that one might worry about the role of chemical bonding in this picture.

"*Self-assembly*", although having a much longer history, became a new mode of both conceptualizing chemical processes and doing synthesis in the 1980s when chemists noticed that, under certain experimental conditions, complex series of reaction steps take place, leading to larger and more complex molecular structures than would be available by classical chemical synthesis. In self-assembly, the intermediary product of the first reaction step triggers or catalyses the second one which in turn favors a third step, and so on, in a rapid series of reactions leading to a complex product. It is the art of the chemists, as they see it, to initiate the series of steps by favorable conditions that direct the entire process toward the desired nanoscale product. Besides conventional conditions, the crucial starter can be a "template" molecule that functions like a mould or a model for the self-assembly of components. The term "self-assembly" already reveals that chemists consider a second agency to be at work here that is usually referred to as "Nature". And since they find many models of such processes in living beings, they frequently describe the approach of "chemical synthesis by self-assembly" as based on "learning from Nature" or "biomimetic". This is only one of many instances in which that fundamental notion of alchemy, indeed its basic technological paradigm, is still influential in today's chemistry (Schummer 2003).

The difference between the two technological paradigms could not be greater. "Atom-by-atom-manipulation" highlights the virtues of high-precision and total human control over the whole material process ("nature"), which would require complete deterministic understanding of all possible events in classical mechanical terms. "Self-assembly" focuses on virtually selected starting conditions and relies, for the rest, on the virtues of "Nature". Although an understanding of "self-assembly" in terms of chemical thermodynamics and kinetics is important, a complete deterministic understanding is usually regarded beyond reach, and not necessarily required for synthetic success. In fact, many chemists consider "self-assembly" smarter and superior to the almost two century old approach of classical chemical synthesis, which is a kind of "atomic-group-by-atomic-group-manipulation" based on the non-mechanical theory of chemical structures and reaction mechanisms.

Since both technological paradigms play a leading role in current nanotechnology, it is hard to see how research approaches guided by such opposing views could ever merge toward interdisciplinary collaboration. The recent Drexler-Smalley debate, their mutual misunderstandings and mis-

conceptions, provides an excellent example of how chemists and mechanical engineers can be talking at cross-purposes, each relying on their own technological paradigm.<sup>12</sup> The debate illustrates that metaphysical notions rooted in history and disciplines pose strong barriers not only to interdisciplinarity and mutual understanding. They can also cause hostility if each party denies the other the expertise due to the “wrong” technological paradigm.

## Conclusion

Given the need for interdisciplinarity in nanoscale research, the current situation is not very encouraging. Despite their multi-disciplinary appearance, newly launched “nano journals” contain hardly more interdisciplinary research than typical mono-disciplinary journals. Obviously, interdisciplinarity is much more difficult to achieve than multidisciplinary. In this paper, I have pointed out two of the cognitive reasons. First, the widely proclaimed common ground—the nanometer scale of objects—is too weak to integrate different disciplinary perspectives. Second, nanotech visions that are meant to orient researchers towards common goals refer to technological paradigms that are rooted in different disciplines and may, in contrast, pose strong barriers to interdisciplinarity. My conclusion is that the present situation requires serious thinking and rethinking about the cognitive conditions and possibilities of interdisciplinarity in nanoscale research.

My critical conclusion comes at a time when political ambitions, at least in the US, further extend the reach of interdisciplinarity (Roco & Bainbridge 2002). Nanotechnology, wrongly considered a homogenous field, is supposed to be one of four fields that combine to form the future scientific landscape, the other three being biotechnology, information science, and cognitive science. The result shall be a super-interdisciplinary structure of the whole of science, including technology, social sciences, and the humanities—a new unity built on the pragmatic goal of improving human performance instead of the dismissed idea of physicalistic “reductionism”. Although that vision complies with “anti-disciplinary” and anti-reductionist ideas advanced in recent science studies, the actual situation in current nanoscale research gives rise to serious doubts (see also Schummer 2004). Instead of discussing such Big Pictures, detailed philosophical work is needed to understand both the chances of and the barriers

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<sup>12</sup> See *Chemical & Engineering News*, 81 (2003), No. 48, pp. 37-42 [<http://pubs.acs.org/cen/coverstory/8148/8148counterpoint.html>]

ers to interdisciplinarity caused by the similarities and differences between the disciplines.

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# CHEMISTRY OF THE STRATOSPHERE: METROLOGICAL INSIGHTS AND REFLECTION ABOUT INTERDISCIPLINARY PRACTICAL NETWORKS

GWENAËL BERTHET  
AND JEAN-BAPTISTE RENARD

## Introduction

The discovery of an “ozone hole”, firstly above Antarctica in 1985 (Farman et al., 1985) and then above the Arctic in the 90s (Salawitch et al., 1993), has motivated the creation of a dedicated scientific community. The consequence of such ozone losses was found to be hazardous for the Earth environment. Stratospheric ozone, in the 10 - 50 km altitude range with maximum concentrations between 15 and 25 km depending on latitude, acts as a shield against natural UVB radiations. A decrease of the thickness of this protective layer would increase the UVB radiation at ground, which could be dangerous for the biosphere. These ozone losses, primarily resulting from the chlorofluorocarbons (CFCs) produced by human activity, were amplified by the strong volcanic events at the end of the 20<sup>th</sup> century.

Soon after these discoveries, a large number of governments funded major international campaigns of observations, including several satellite programs. The famous Montreal Protocol (1987) initiated the progressive replacement of CFCs by other constituents, the Hydrochlorofluorocarbons (HCFCs) and the Hydrofluorocarbons (HFCs). HCFCs deplete much less ozone per kilogram emitted than CFCs, while HFCs are basically non-ozone depleting gases. More constraining amendments were then applied for the use of these chemical compounds.

The stratospheric chemistry was not well understood at the beginning of the 80s. Since then, strong improvements have been achieved by the various scientific communities that have worked together. This has been

possible thanks to the available funding and manpower, and to a very efficient coordination of various activities.

## 1. Stratospheric Ozone

Stratospheric ozone is produced when molecular oxygen  $O_2$  is photodissociated after absorbing photons having wavelengths below 240 nm.  $O_2$  is thus converted to atomic oxygen O. The oxygen atoms combine with molecular oxygen to produce ozone molecules; this reaction is characterized by heat production, explaining why the temperature gradient is positive in the stratosphere.  $O_3$  absorbs light between 200 and 310 nm; then the ozone molecule is broken to produce  $O_2$  and O. The total amount of ozone is regulated through photochemistry and recombination processes.

Ozone can be destroyed by some radicals acting as catalysts: OH, NO, Cl and Br (we adopt here the quotation commonly used by atmospheric scientists). Although hydrogen and nitrogen radicals have mainly a natural origin, chlorine and bromine radicals are mainly the result of human activities. These elements are contained in stable organic compounds that can easily reach the stratosphere and stay several tens of years even if they are produced at ground level.

Under UV radiations, CFCs are photodissociated to produce chlorine atoms, which leads to the formation of the HCl and ClONO<sub>2</sub> stable chlorine reservoirs. During the polar winter, the stratosphere encounters very low temperatures, typically below -80°C. Such conditions result in the formation of polar stratospheric clouds (PSCs); PSCs are composed of nitric acid or sulphuric acid and water. At the end of the winter and at the beginning of spring, in presence of sunlight, the chemical compounds produced from uptake of HCl and ClONO<sub>2</sub> and heterogeneous chemical reactions at the surface of PSCs are photodissociated to release the free radicals Cl and ClO. Also, the sedimentation of PSCs leads to the partial removal of the nitrogen reservoir species HNO<sub>3</sub>. This process, called denitrification, strongly reduces the formation process of nitrogen oxides; ClO cannot be converted into its reservoir species ClONO<sub>2</sub>, thus sustaining the destruction of ozone.

The chemical scheme involving the  $Cl + O_3 \rightarrow ClO + O_2$  and  $ClO + O \rightarrow Cl + O_2$  reaction destroys ozone. Cl, recycled from the second reaction, acts as a catalyst. The result is  $O_3 + O \rightarrow 2 O_2$ . Thus, a single chlorine atom can destroy  $10^5$  ozone molecules. Other catalytic cycles involving chlorine radicals and nitrogen radicals, bromine radicals and hydrogen radicals, play a more or less significant role in the ozone destruction depending on the altitude. A cycle similar to the one of

chlorine species involves the Br and BrO radicals, and participates to about 25% of the ozone destruction. Although the bromine species concentrations are ~200 times lower than chlorine species, they are individually more efficient to destroy ozone.

PSCs disappear as the stratosphere gets warmer. This occurs in November for the Antarctic stratosphere, and is more irregular during spring for the Arctic stratosphere. Depending on the year, the Arctic ozone loss strongly varies, although being smaller than the one above Antarctica. This is due to the fact that stratospheric temperatures in the Arctic are warmer (typically of about 10°C) and less in favour of PSC production. After the spring stratospheric warming, the ozone recovery is onset from the mixing of polar air masses and mid-latitudes air masses rich in ozone.

The situation is more complex during major volcanic eruptions, where a large amount of liquid sulphate aerosols are formed in the stratosphere. These aerosols participate in additional ozone destruction (Brasseur et Granier, 1992) and to a decrease of Earth surface temperatures for several years (Solomon et al., 2011).

Two different phenomena occurred at the end of the last century: the increase of the CFCs in the stratosphere and two major volcanic eruptions: El Chichón in 1982 and Mount Pinatubo in 1991 (Russell et al., 1996; Deshler et al., 2003). Then, a fast increase of ozone loss was observed at the beginning of the 90s; some scientists released alarmist anticipations for the following years and decades. Also, it was suspected that global ozone was decreasing at all latitudes.

The seasonal ozone losses observed in the Antarctic stratosphere (Figure 1) were strong enough to take worldwide political decisions, beginning with the Montreal protocol. In parallel, all the necessary funding, technical needs and manpower were provided to better document the ozone loss phenomenon, and to better understand the involved chemical processes. The main objectives were to be able to distinguish between the natural origin (volcanoes) and the human origins (CFCs and bromine species), to follow the consequences of the Montreal protocol, and to be able to predict when ozone will recover its original level (before the industrial period). Today, we are observing unambiguously in the atmosphere a decline of the anthropogenic species that destroy ozone. Nevertheless, ozone loss will continue for several decades due to the lifetime of these chemical species in the stratosphere. From modelling works, we expect to recover the original ozone levels in the mid-XXI<sup>st</sup> century (Newman et al., 2006).

All these new scientific results have motivated the association of different teams that perform laboratory chemistry measurements,

spectroscopy, modelling works, and that develop instruments at ground level, onboard aircraft, balloons and satellites. Coming from different countries, all these scientists have worked together using the same scientific language and have developed in a short time all the necessary tools for these studies. In few years, the knowledge of the stratospheric and upper troposphere chemistry strongly improved. Such progress would have been impossible without scientific synergy, i.e. only from presentations of individual research work in scientific papers or during colloquiums.

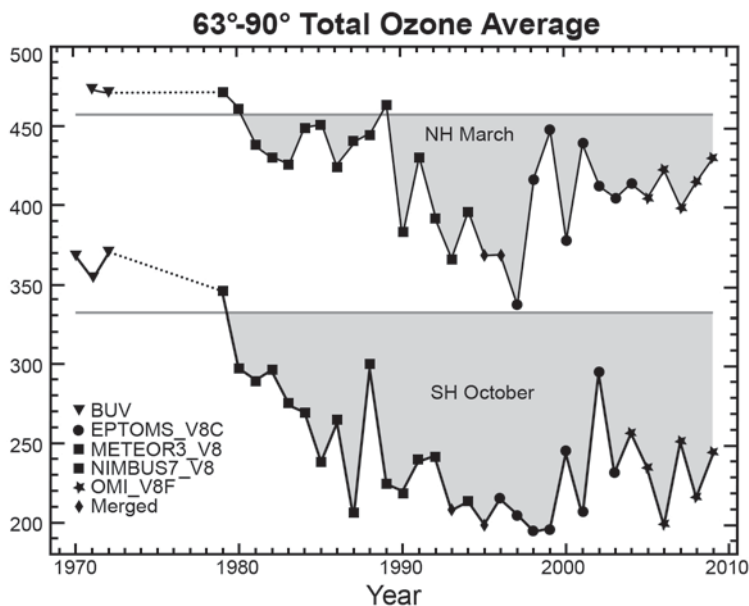


Figure 1: Averaged vertical columns of ozone from various satellite data, for the Northern polar region (NH) and the Southern polar region (SH); from: Scientific Assessment of Ozone Depletion: 2011, World Meteorological Organization

## 2. Techniques of Measurements, their Constraints and their Limits

A main difficulty in stratospheric chemistry studies is to properly measure different key chemical species together with their spatial and temporal variability. Another issue to deal with is that typical concentrations from one species to another can differ over several decades.

The ozone hole is observed between 10 and 30 km in altitude over a certain horizontal area which is likely to significantly fluctuate over the season; thus we cannot use only isolated ground-based measurements of vertical columns of ozone (i.e. the total amount of ozone above the instrument), as well as for other species, even if this type of measurements is useful. It is needed to observe the phenomenon as close as possible within the stratosphere. Its spatial and temporal evolutions must be adequately captured and monitored, mainly from space. The measured concentrations are very low: several ppmv (one molecule for  $10^6$  air molecules) for ozone, several ppbv (one molecule for  $10^9$  air molecules) for nitrogen and chlorine species, and several pptv (one molecule for  $10^{12}$  air molecules) for bromine species. Finally, the PSCs have different compositions depending on the temperature and their formation processes.

There is no “universal” technique to measure the ~50 species involved in stratospheric chemistry. It is necessary to develop different techniques depending on the targeted compounds. All the atmospheric observations must be coordinated and combined in order to be compared to modelling works.

We will not present here a detailed list of all the measurement techniques but will specifically focus on absorption spectrometry, which is one of the main methods used to retrieve the atmospheric composition. The principle is simple: concentrations of the atmospheric compounds are derived from their absorption lines using the Beer-Lambert law which directly relates the depth of these lines to the number of molecules along the line of sight (if the absorption lines are not saturated). To be able to reach the required accuracy, flux variations of the order of  $10^{-4}$  must be detected with instruments having an adequate spectral resolution. For example, the spectral resolution must be of about 0.5 nm in the visible domain and of about  $0.03\text{ cm}^{-1}$  in the mid-infra-red (around  $10\text{ }\mu\text{m}$ ). The observations can be conducted by remote-sensing techniques, using natural light sources (Sun, Moon, Stars, stratospheric emission), mainly from satellites and from balloons; this technique is called “occultation method” (e. g. Renard et al., 1996). Observations can also be made using in situ techniques characterized by a light source (such as laser diodes) inside the instrument and an air-open cell (Moreau et al., 2005), obviously conducted from aircraft and balloons.

Thanks to national and European fundings, strong instrumental improvements were achieved in a few years. Most of these instruments were mounted onboard balloons and aircraft. Scientific and technical teams coming from other domains in physics and chemistry joined the

stratospheric ozone studies, sometimes providing new techniques of observations. A similar approach was conducted in the United States.

The European, US, Japanese, Canadian and Swedish space agencies also developed satellite platforms specifically dedicated to stratospheric ozone chemistry studies. At the European level, the biggest environmental satellite built by the European Space Agency, Envisat (Figure 2) carried three instruments devoted to this scientific issue (the seven other instruments were dedicated to Earth observation). Satellite instruments are able to perform measurements from an altitude of several hundreds of kilometres; thus, remote-sensing spectrometry is the only existing technique to determine the abundance of the species in the upper atmosphere.

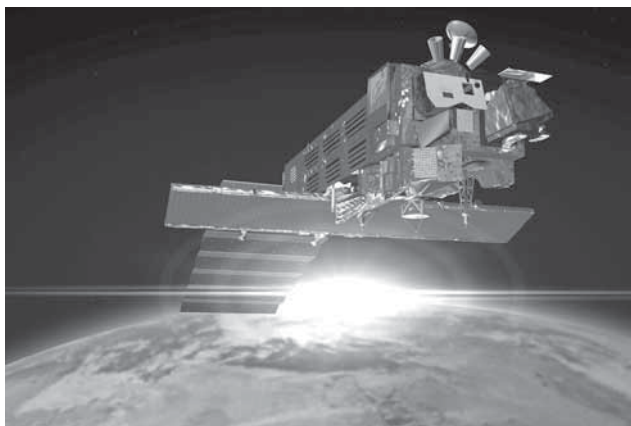


Figure 2: The Envisat European satellite (European Space Agency, <http://www.esa.int/>)

It is necessary to use laboratory spectroscopic data, called absorption cross-sections, to interpret the spectra measured by all these instruments and subsequently derive the species abundances from the Beer-Lambert law. The absorption cross-sections of a given molecule are related to the absorption probabilities of a light at given wavelengths and therefore reflect the spectral lines. Up to the 90s, the cross-sections were not so accurate and were sometimes measured tens of years before. It was then necessary to determine more accurately these cross-sections so as to satisfy the scientific requirements in terms of accuracy and spectral resolution of the teams who perform the atmospheric measurements.

Cross-sections are difficult to measure. We must know the exact concentration of the chemical species inside the laboratory cell. Also, spectrometers must be of high quality with accurate wavelength calibration (in particular when the spectral signature of the studied molecule exhibits thin lines). The targeted molecules are produced within the cell by chemical reactions; thus it is necessary to know their production mode and the reaction rate constants also determined in the laboratory. The consequence is that different teams must work together and sometimes by iterative processes. It is also necessary to use very clean cells, to avoid the possible presence of contaminants which are likely to chemically react or produce unexpected absorption lines. Most of the time, the chemical reactions and cross-sections are dependent on temperature and pressure. It is then necessary to reproduce typical stratospheric conditions in laboratory which is not obvious for temperatures below 200°K. Figure 3 presents the NO<sub>2</sub> cross-sections obtained at the Bremen University (Germany) by Voigt et al. (2001).

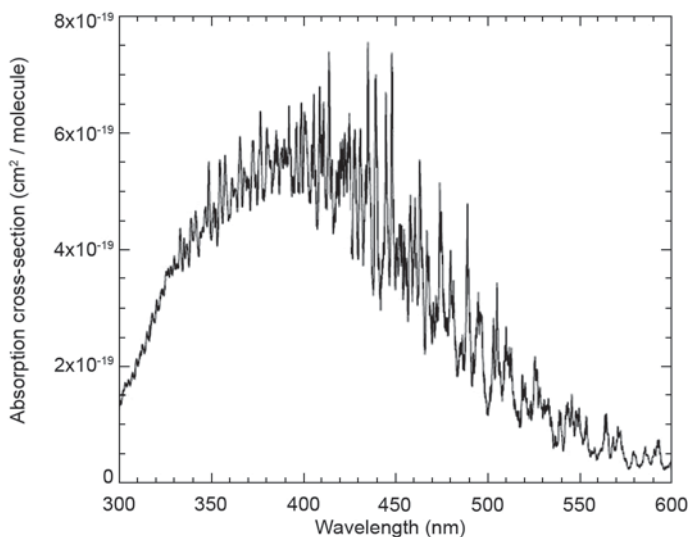


Figure 3: NO<sub>2</sub> cross-section at 223°K, in the visible domain (Voigt et al., 2001)

Inevitably, all these laboratory measurements have some uncertainties. Different teams in the world perform this type of measurement. The comparison of these various sets of data can allow the scientists to point out some possible biases in the individual records. A good accuracy is



achieved when the various data sets exhibit a difference typically below  $\pm 10\%$ . Databases widely open to the scientific community and without access restriction are now available, as for example HITRAN (<http://www.cfa.harvard.edu/hitrان>).

If the stronger absorption lines for the main atmospheric species are now well determined (ozone, nitrogen oxides, chlorine species, bromine species, iodine species), some uncertainties remain in particular in the infrared spectral domain where a large number of thin lines are present, especially from ozone and water vapour. If the cross-sections, rather used on restricted spectral ranges to interpret the observations in the stratosphere, are inaccurate or not available at stratospheric temperatures, species concentrations retrieved at different altitudes could be somewhat erroneous.

From comparisons between atmospheric measurements of the spatial distribution of the species and modelling work, significant discrepancies have been recurrently detected. The ensuing question would be: what is wrong? Is it the measurement or the modelling work? Before concluding that the knowledge of the stratospheric chemistry needs improvements, all the data analysis processes and the cross-section values must be re-examined. This work needs coordination between the teams who operate the instruments in the atmosphere and the laboratory scientists. Finally, if the discrepancies are confirmed, one could conclude that our knowledge of the stratospheric chemistry is partly erroneous. Then, the chemical reaction rate constants must be re-analysed in the laboratory and some new channels for production/destruction of the species must be searched for. It must be noticed that other important parameters, as computation of transport (in other words “atmospheric dynamics”) of species in the modelling works, could be re-analysed and improved. Nevertheless, artificial detections from atmospheric observations are still possible...

Two examples coming from studies in our team (LPC2E-CNRS) can be given. The first one is on the detection of concentration enhancements of  $\text{NO}_2$  in the winter-time high-latitude lower stratosphere below 20 km, while the model outputs give zero concentration. Such detections were obtained by balloon-borne instruments performing remote sensing measurements. Satellites observations are also somewhat likely to exhibit such enhancements, although satellites measurements are considered to be inaccurate at these altitudes (Renard et al., 2008). Several hypotheses have been proposed to explain such unexpected  $\text{NO}_2$  concentrations, as the one involving unknown heterogeneous reactions with solid aerosols (Lary et al., 1997). The answer was obtained by the comparison of measurements performed a few days apart in similar air masses, using a balloon-borne

remote sensing instrument (SALOMON), an in situ balloon-borne instrument (SPIRALE) and the data obtained by the satellite instrument GOMOS onboard Envisat (Figure 4). The in situ measurements provided a zero value, in agreement with the modelling outputs REPROBUS (Lefèvre et al., 1994). In fact, the detected high  $\text{NO}_2$  concentrations were originating from a bias inherent to remote sensing techniques. Indeed, it has been found that local concentration inhomogeneities along the instrument lines of sight are likely to induce artificial enhancements in the vertical profile retrieval process (Berthet et al., 2007). This result shows that balloon and satellite data must be used cautiously in case of a dynamically perturbed stratosphere, namely when air masses of different origins are close together or during their mixing process (for instance during and after the break-up of the ozone hole which mixes with mid-latitude air masses).

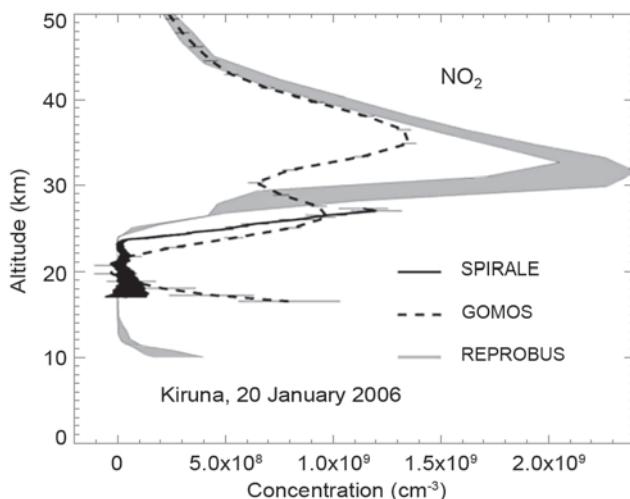


Figure 4: Comparison between the GOMOS instrument (onboard the Envisat satellite), the in situ balloon-borne instrument SPIRALE, and the modelling outputs from the REPROBUS model (Berthet et al., 2007)

The second example deals with the OBrO species, involving balloon, laboratory and modelling teams. Unknown spectral lines were detected from spectroscopic laboratory measurements and were attributed to OBrO (Rattigan et al., 1994), although the production mode was unknown. Soon after the release of this discovery, the spectral signature of OBrO was searched for in atmospheric measurements. Our team claimed the possible

detection of this species that could be the main night-time stratospheric bromine species (Renard et al., 1998). But this detection was in total disagreement with modelling outputs giving a zero value for OBrO. It was a situation where all the measurement techniques were pushed to their limits. The cross-sections are inaccurate, the production mode and the constant rates are unknown, and the absorption lines in the stratospheric measurements are close to the instrument detection threshold. It is commonly assumed that BrONO<sub>2</sub> is the main night-time bromine compound but this species is not expected to be detectable from typical instruments using absorption spectrometry techniques. After re-analysis of the measurements by the MIPAS (onboard the Envisat satellite) infrared spectrometer, a team has announced for the first time the stratospheric detection of BrONO<sub>2</sub> (Höpfner et al., 2009), invalidating our OBrO detection. Nevertheless, this new analysis could exhibit a bias that would rule out the reality of this BrONO<sub>2</sub> detection. Thus, stratospheric night-time bromine chemistry remains an open question, although discussions on this subject are less active at present since no new elements have been released.

### **3. Measurement Campaigns and Interpretation by Modelling Outputs**

Only a few instruments dedicated to stratospheric chemistry studies were available in the 80s before the ozone hole discovery and suffered from a lack of accuracy. At the end of the 80s, due to a sustained international effort, an increasing number of instruments with better accuracy became available, sometimes with new and highly expensive techniques of measurements.

In Europe, the European Commission was a major actor for funding field campaigns at different latitudes and for funding a coordination process to collect and compile all the data. The “European Ozone research Coordination Unit” started its activities at Cambridge University (United Kingdom) in April 1989. Thus, from 1992 to 2009, six main campaigns of measurements were organized. Observations were conducted mainly in the Arctic, because this region offers much more facilities than Antarctica and was poorly studied at this time. Also, studies at mid and tropical/equatorial latitudes became rapidly necessary because pollutants present in the Polar Regions originate from these areas as a result of the global atmospheric circulation.

These campaigns combined observations from aircraft in the lower stratosphere (including an aircraft that can reach an altitude of 22 km) and

from stratospheric balloons up an altitude of 40 km. The balloons were mainly launched by the French space agency CNES. These kinds of observations provide very accurate concentration measurements but only over a short time, typically several hours, and for a limited geographical extent, at least several hundreds of kilometres. These observations were coupled to those obtained by satellite instruments which are typically ten times less sensitive but provide large-scale spatial coverage. Some satellites can be operated for more than 10 years and can provide a global coverage of Earth atmosphere at the day scale. Combining all these observation approaches allows the scientific community to study both fine processes and long-term trends of the species. The same approach was used in the US, in particular with the NASA American space agency as the main partner.

All these measurements are compared to modelling outputs. The objectives are to test the current knowledge in stratospheric chemistry that is represented by numerical equations and to possibly identify new physical and chemical processes. Several 4D models (4D means the 3D repartition of the Earth atmosphere and its evolution with time) have been developed; the modelling outputs are released from several weeks to several months after the date of observations. Some modelling outputs are available on the internet, as the REPROBUS outputs (Lefèvre et al., 1994). In particular, the observation data and modelling works funded in France can be found on the ETHER database (<http://ether.ipsl.jussieu.fr>). These models are developed in synergy by physicians and chemists who are familiar with sophisticated mathematical tools and multiple equations. The meteorological and chemistry parts in the models are often structured in separate modules that interact together. For the chemistry part, the equations represent the chemical reactions between the various species, which could be interlinked. Laboratory chemistry teams provide the reactions channels and the rate constants. These values must be frequently updated, thanks to an increasing number of accurate laboratory protocols and measurements. Nevertheless, some errors and uncertainties remain in these experimental data, which is problematic. They must be taken into account when interpreting the output modelling.

Epistemology studies could help to better evaluate the meaning of laboratory experimental errors. In particular, they could be valuable to make the scientists cautious about the use of the most recent datasets. Such studies could reflect that recent data do not automatically mean better data, as shown by large number of examples in the past. Also, investigations could be conducted on the meaning of the measurement procedure. Thus, a study about how to perform measurements in a complex medium could be

carried out. Such approach could help to better evaluate the heuristic role of modelling works and their integration in a large research program. Finally, the study could help to better consider instrumentation as the centre of research approaches.

The comparison between atmospheric measurements and modelling outputs are conducted both by experimental and theoretical teams. They must be aware of the limits of the models. Some of the discrepancies between measurements and modelling outputs could be also linked to numerical constraints and computer limitations (hypothesis or simplifications, digitization, spatial and temporal resolution) but they are difficult to well identify. Nevertheless, it is always necessary to simultaneously re-analyze stratospheric measurements for which some biases are possible, as presented above, and to perform new measurements of laboratory rate constants and cross-sections used for the modelling work. This last point must be conducted cautiously. As an illustration, at the end of the 2000s, new chlorine chemical reaction parameters from laboratory studies (Pope et al., 2007), in total disagreement with a large number of previous studies, were not accepted by the scientific community and were considered to be erroneous (WMO, 2010). With this new dataset, model outputs gave unrealistic results concerning the stratospheric ozone destruction. It is interesting to notice the reactivity of the scientists just after the publication of these new data in 2007. New sets of measurements were intensively obtained between 2007 and 2009 by different international teams. In particular, a specific Arctic campaign of observations in 2010 was funded by the European Commission. This strong reactivity reminds one of the reaction just after the ozone hole discovery, of course at a smaller degree. Finally, this episode has given a new interest to stratospheric chlorine chemistry and has allowed the scientific community to better quantify the parameters linked to the ozone loss in the modelling works.

Finally, new chemical reaction channels that were thought to be of less importance could in fact be stronger than expected (this occurs sometimes). Thus, all the studies are carried out in strong interactions between the various teams; atmospheric measurements can motivate new chemical studies in laboratories, but also some laboratory studies can lead to the development of new stratospheric instruments and improvements of models.

International colloquiums are regularly organized to present all these results. The scientific topics are pluridisciplinary, involving chemists, physicists, modelling teams, and mathematicians for sophisticated data reduction algorithms. In particular, every 4 years, the “Quadrennial Ozone

Symposium” is the place to assess the work on stratospheric ozone chemistry and dynamics.

#### 4. After the Ozone Hole

Such a demanding international effort cannot be sustained indefinitely. After 20 years of intensive studies to eventually be able to determine the ozone trend with an accuracy of about one percent, it is now possible to announce that ozone losses are globally stopped and that the recovery seems to have started. This good news has validated the political and economical approach of the Montreal protocol. This is an interesting example of how the political world must react against a worrisome situation. The reality of ozone losses was accepted by the whole scientific community, even if some short-time predictions were too alarmist due to a bad estimation of the role of volcanic aerosols in the observed ozone trend.

From a scientific point of view, all these years of measurements have allowed us to understand that stratospheric chemistry is more complex than expected (which occurs often in science). In fact there is a need to continue the ozone studies but this argument is too weak to obtain again the huge funding and the manpower obtained in the past. Also, new scientific interests are emerging, as the global climate warming and tropospheric pollution. Thus, it will be unfortunate if all these different scientific communities that have worked together in the past set off to work in their original domains.

These links between the different teams and institutes (and institutions) are strong enough to be able to maintain this pluridisciplinary approach. The study of the stratosphere is now extended to the lower troposphere, with particular focus on the pollutant transport and the water vapour cycle, to better understand the interaction between climate and atmospheric chemistry evolution. In particular, dynamics and chemistry of the tropical and equatorial atmosphere are not well understood and new efforts are expected to better document these regions. Of course, the number of measurement campaigns will be fewer than before but actions developed for the ozone hole will be maintained.

New studies concern also the mesosphere and the high energy phenomena (blue jets, sprites, elves) and their consequences for atmospheric chemistry. These phenomena occur above strong thunderstorms and are characterized by electric discharges from the tropopause to the mesosphere, in the 10-70 km altitude range (e. g. Van der Velde et al., 2006). Gamma-ray flashes are sometimes associated with these events. The role of laboratory chemists and modelling teams is to establish the chemical

reactions that can occur during such events. This scientific domain is rapidly growing, with a new pluridisciplinary approach including new scientific communities in addition to those already working together on ozone chemistry.

The main problem will be the lack of satellite measurements dedicated to stratospheric chemistry in the following years, since no major European satellite is planned at present; the efforts of the space agencies mainly concern the troposphere and the greenhouse gases  $\text{H}_2\text{O}$  and  $\text{CO}_2$  at present. Then, more efficient instruments that can partly replace the satellite instruments could be mounted onboard aircraft and balloons. Two approaches are now developed. The first one is to build complex instruments with a better accuracy and that can measure a larger number of species during longer balloon flight sessions. The second one concerns the development of low cost and miniaturized instruments, for the measurements of one or two species, which can be extensively launched under small (meteorological) balloons from a large number of locations.

For laboratory measurements, a major issue deals with heterogeneous chemical processes on solid aerosol surfaces (frozen or not-frozen particulates). Indeed, some strong uncertainties remain on the reactivity of some species, mainly nitrogen compounds, with the aerosols. It seems that some unknown reactions are still waiting to be discovered. This approach could explain some of the permanent discrepancies between measurements and model outputs in the lower and middle atmosphere. A large number of laboratory chemistry teams are now involved in these studies (e. g. Nozière et al., 2009); their work will lead to new atmospheric instruments to be able to monitor the evolution of some species and the aerosols instead of “one shot” measurements during campaigns. One objective is to better understand the role of human activities on the ambient air quality and thus to be able to theoretically predict how the atmosphere will react to some pollution events. Finally, some laboratory atmospheric chambers of several meters in diameter are now available to reproduce the relevant atmospheric conditions. They will allow us to study the temporal evolutions of the species over a long period of time.

## Conclusion

The strong efforts following the discovery of the ozone hole have allowed the scientific community, in only a few years, to greatly improve knowledge in atmospheric chemistry, to develop a large number of efficient instruments for laboratory and atmospheric measurements, and to have powerful modelling tools.

The Earth's atmosphere must not be studied through separate research domains (species, altitudes, geographical regions, etc.). The atmosphere is a whole subject of research with its different parts (troposphere, stratosphere, and mesosphere) linked together. Thus, new topics of research are emerging, as the study of tropical regions, and connect new scientific communities, as the one on atmospheric electricity and on the ionosphere, to the previous ones. There are now several international communities who speak the same scientific language and know how to put their tools in common. In particular, chemists are thoroughly involved in their laboratory measurements but also in theoretical work and in the development of new atmospheric instruments. It is necessary to sustain these communities, which implies the need to establish new comprehensive projects to get large financial support. Also, the different methods and procedures for funding, that the different teams used in the past, must be grouped together. Thus, the methodologies developed during the ozone hole story could be maintained and developed for the new scientific objectives that will emerge in atmospheric studies; these studies can be related to the consequence of human activities or to the "pure" knowledge of the atmosphere.

Works on history of chemistry and atmospheric sciences will also be necessary to better understand the scientific and political challenges and the outcomes of the ozone hole episode. This will allow us to analyse serenely the whole story. In the future, such works could prevent the appearance of methodological errors that inevitably occur when new exciting and critical scientific subjects emerge.

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# CURRENT RELATIONS BETWEEN CHEMISTRY AND BIOLOGY: THE EXAMPLE OF MICROARRAYS

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## Introduction

It would be artificial trying to completely separate biology from the other sciences. There has always been a close relationship between biology and chemistry as well as maths and physics.

Here are some examples to prove our point.

Louis Pasteur was a chemist (by training) and studied chemical problems (the chirality of molecules) at the beginning of his career. The study of molecular dissymmetry lies at the origin of the intuitions that led him to the field of microbiology with the known success.

Jacques Monod is one of the founding fathers of molecular biology. During the studies that led him on to win the Nobel Prize, he asked Melvin Cohn for help. The latter was a biologist who had a better grasp of chemistry and who synthesized thiogalactosides for the laboratory's need, including isopropyl  $\beta$ -D-1-thiogalactopyranoside, which played a fundamental role in the elucidation of the functioning of the lactose operon (Monod, 1966).

On the other hand, research at the English biometric school on the mechanisms of evolution and selection has led to numerous statistical concepts, which are constantly applied to all the branches of sciences, for example the linear regression used by Francis Galton in 1886 and the correlation coefficient used by Karl Pearson in 1896 (Orr, 2005).

These bonds between the various disciplines are even stronger in molecular biology because it was born from a fusion of biochemistry and biology at the beginning of the 1960s. This idiosyncratic cultural mixture shows in the curriculum of its young researchers. To take up Erwin

Chargraff's aphorism (National Medal of Science 1974): 'Molecular biology is biochemistry without a licence'.

In France of the 1960s less than a third of the young researchers who turned to molecular biology came from the field of biology (BSc in Natural Sciences, medical doctors or vets). The rest had followed an initial training in physics or chemistry. This over-representation of non-biologists was the result of a deliberate policy by the "Comité de biologie moléculaire de la DGRST" (Polanco, 1990).

Over the years and following reforms, maths, informatics, physics, chemistry and biochemistry have gained an ever-increasing importance, currently representing about 40% of a typical life sciences syllabus.

## **1. The Example of Microarrays**

To look at the current relations between chemistry and biology, we have chosen the history of microarrays for two main reasons: 1) they have revolutionized the way problems are tackled in the entire field of biology and 2) it is a technique that started out firmly in the realm of the biologists and ended up just as firmly in that of the chemists (and physicists).

It is also a pedagogic example that fits in with the purpose of this book:

- It illustrates the specificities of the biologists' approach compared to the working methods of chemists;
- it represents a case where the same problem can be solved by both, a biologist's or a chemist's approach;
- the two different solutions currently co-exist in the labs;
- the industrialization of the microarray production has not led to the disappearance of their "in house" fabrication in biology labs;
- the criteria for choosing between the two solutions are clear. Most notably, it is only the chemist's approach that can easily be scaled up for an industrial production.

## **2. Some Typical Working Methods in Biology**

In order to appreciate the changes that were brought on in biology, it is important to be familiar with the classical working methods in a biology lab. Some of these techniques actually formed the basis for the development of microarrays.

The typical workflow is as follows:

1. You obtain sufficient biological material to carry out your study, generally by growing cells on a suitable substrate.
2. You extract the nucleic acids (either DNA or RNA, depending on the study's aim).
3. If the quantity of nucleic acid proves insufficient, you produce a great quantity of the fragments of interest using a procedure called PCR (polymerase chain reaction). One talks of RT-PCR when working from RNA. The PCR was invented by a biologist turned chemist (Nobel Prize in Chemistry 1993) (Saiki *et al.*, 1985; Mullis, 1993).
4. The DNA is cut at precisely defined sequences using restriction enzymes (discovered by biologists who won the Nobel Prize in Medicine in 1978) (Smith & Welcox, 1970; Arber, 1978; Nathan, 1978; Smith, 1978).
5. The DNA fragments are then separated according to their size by electrophoresis, a method initially invented to separate the proteins present in the serum (Nobel Prize in Chemistry 1948) (Tiselius, 1937, 1948).
6. The DNA fragments or proteins are then marked in order to detect them in further experiments. The techniques available are listed below.

It should be mentioned that biologists study macromolecules, which are present from the start. Their merit lies in being able to get the cells or specific enzymes to produce sufficiently large amounts of the desired molecule, purify (directly or indirectly as in the case of the PCR) and then mark it. As opposed to chemists, they do not synthesize from scratch or through semi-synthesis.

Of course biologists need chemicals to carry out their work and they will order them from specialized chemical suppliers like industrial kits to extract and mark nucleic acids. However, when required, they are able to prepare the molecule they need themselves, as it was the case with restriction enzymes in the 1970s. The University of Edinburgh was home to the “restriction endonuclease club”; to join, biologists had to purify a new restriction enzyme (Greene *et al.*, 1978; Southern, 2005).

In any case, biologists regard it as fundamental to master the procedures listed above and to carry them out in their labs.

The insert describes how biologists build a genomic library, a procedure that precedes the study of an organism and is also necessary for the production of spotted microarrays (see below).

### 3. The Concept of Molecular Marking

It is an essential one in biology because most often the molecules studied are difficult to identify with the necessary precision using the common chemical or physical techniques. The UV spectrum of a DNA fragment, for example, is the same regardless of the nucleotide sequence. Now, it is precisely this sequence, which encodes the genetic message. Furthermore, a number of proteins do not have any catalytic property or one that can only be measured with difficulty.

The marking techniques described below are important in their own right but opened the way for the development of microarrays.

Albert Hewett Coons (MD) was the first to develop immunofluorescent techniques for labelling antibodies in the early 1940s (Coons *et al.*, 1942). He continued his work after the war with the help of Louis Fieser, a chemist. The technique allows detecting the presence of a given molecule *in situ* provided it has antigenic properties (Mellors, 1968). The technique was further developed throughout the 1950s and 60s. Albert Hewett Coons received the *Albert Lasker Award for Basic Medical Research* (1959).

Immunofluorescence is ill suited for quantitative measurements. This problem was overcome through the development of radioimmunoassays (or RIA), a technique that is both, sensitive and precise. The technique was invented by two medical doctors in the 1950s, Rosalyn Yalow and Solomon Aaron Berson (Yalow & Berson, 1960). It consists in measuring the decrease in radioactivity of the antibody-radioactive antigen complex when adding the extract under study. Rosalyn Yalow was awarded the Nobel Prize in Medicine 1977 (Berson had already died by this time) (Yalow, 1977).

At the end of the 1960s and beginning of the 1970s researchers found a way to avoid using radioactive material by measuring the catalytic activity of an enzyme which had been attached to the antibody (enzyme immunoassay or EIA; enzyme-linked immunosorbent assay or ELISA). The two techniques were invented simultaneously and independently by two teams: (1) Anton Schuurs and Banke van Weemen for EIA (Van Weemen & Schuurs, 1971), and (2) Peter Perlmann and Eva Engval for ELISA (Engvall & Perlmann, 1971). It is a technique, which combines the know-how of biology (production of antibodies and enzymes) and chemistry (construction of a hybrid molecule which retains the activity of both).

Equivalent techniques were developed for nucleic acids, replacing the antigen-antibody reaction with the complementarity of DNA strands. The first step was the invention in 1975 of a method to separate DNA

fragments according to their size before transferring them to a membrane and fixing them on it as single strands (a technique known as the Southern blot (Southern, 1975). The extract under study is marked and then allowed to hybridise with the single strand DNA fixed on the membrane. The inventor of this technique, Edwin Southern, is a biochemist and received the *Albert Lasker Award for Clinical Medical Research* in 2005. He also participated in the development of microarrays, which can be seen as generalisation of the Southern blot (Southern, 2005).

Yalow and Berson always refused to patent their RIA technique and until the 1970s biologists used to prepare the necessary materials themselves in their labs. EIA and ELISA, however, have been patented. They are well suited for the manufacturing of industrialized kits, which generally take the shape of 85x125 mm plates with 96 wells containing the fixed antibodies or antigens. One of the advantages of these kits is that they greatly facilitate the automation of tests.

#### 4. Using Fixed Molecules on Solid Supports

Fixing molecules on a solid support in order to facilitate their manipulation during sequential chemical reactions was a technique invented in the 1960s for the synthesis of peptides (the so-called solid phase peptide synthesis (Merrifield, 1963). Its inventor, R. Bruce Merrifield, was a biochemist and received the Albert Lasker Award for Basic Medical Research (1969) as well as the Nobel Prize in Chemistry in 1984 (Merrifield, 1984).

In the 1980s Geysen (a chemist and microbiologist) and co-workers developed the concept further and introduced combinatorial chemistry for the synthesis of peptides in “pools”. Hundreds of (related) proteins could be synthesized at the same time, their position and (amino acid) sequence being decided on *a priori* by the experimenter (Geysen *et al.*, 1984).

There is an important difference between the molecules fixed on a solid support when using ELISA or the techniques of Merrifield or Geysen: in the former, the complete molecule (for example the antibody) is fixed on the support whilst in the latter the peptide is synthesized on the spot or *in situ*. These two different approaches can also be found in the microarrays where the nucleic acid molecules can be either fixed on the support (spotted microarrays) or synthesised *in situ* on a glass plate.

## 5. Get More onto Less: Miniaturization

Frequently the limiting factor in experiments is the quantity of material available for testing.

It was the group around Roger P. Ekins, a physicist, which introduced the concept of microarray by developing microspot fluorescent immunoassays at the end of the 1980s, which required much less biological material than their predecessors (Ekins, 1989; Ekins & Chu, 1991).

A little later the concept of simplification and miniaturization was also applied to the Southern blot leading to the development of DNA microarrays. Every array is made up of ten thousands of regularly distributed spots each containing a very large number of copies of a DNA fragment of known sequence.

### 5.1. Microarrays using *in Situ* Hybridization

#### 5.1.1. The Oxford Group

Southern started out as a protein biochemist and turned to molecular biology at the end of the 1960s, a time when techniques had to be yet invented. He joined the University of Edinburgh, which was one of the very few institutions worldwide to work on genomes. It was home to a rather diverse and very dynamic lot of researchers, who were passionate about technology and the various branches of Science. Southern was member of the “restriction endonuclease club” mentioned above.

Southern was called to Oxford in 1985, where together with the chemist Uwe Maskos, he invented a technique that allowed synthesizing hundreds of DNA sequences simultaneously on a glass support and hybridizing them with nucleic acids in solution. To that purpose Maskos developed a chemical treatment for the glass support, which made it possible to tether one end of the DNA molecule to the glass plate through covalent bonds. He completed his invention by creating a linkage molecule that kept the DNA molecule away from the glass surface, increasing thus its accessibility.

Southern then developed a particularly simple and ingenious piece of equipment to synthesize DNA *in situ* using a physical mask or seal to direct the reagents during synthesis. He used two glass plates. On the first he glued a series of rubber tubes. When pressed against a second glass plate, the array plate, the tubes formed channels. When he applied the reagents at one end of the glass “sandwich”, they diffused to the other end through capillary action and stuck to the array plate because it had been



previously chemically treated to bind nucleic acids. In a first step the plate is divided into four channels (one per nucleotide). This allows fixing the four nucleotides in four parallel stripes on the array plate. The procedure is repeated using a plate with more tightly packed rubber tubes which will divide the plate into four by four channels. The array plate will then contain the sixteen dinucleotides arranged in sixteen parallel stripes. The procedure is repeated until the desired size of oligonucleotides has been obtained. Southern increased the efficiency of this method by rotating the plate by 90° between steps, obtaining thus spots rather than stripes of oligonucleotides and increasing thus the number of different sequences present on the same array plate.

The Oxford Group holds a number of key patents for DNA microarrays. However, it does not commercialize them (Blanchard, 1998; Southern, 2005).

### 5.1.2. The Stanford Group

In 1988 Alejandro Zaffaroni (a biochemist) founded together with J. Leighton Read (a biologist and medical doctor) and Peter G. Schultz (a chemist) Affymax in order to improve the search for pharmaceutically active compounds. Affymax was a start up that worked like a think tank and the founders almost immediately engaged a number of eminent scientists from academia (mostly Stanford) including Joshua Lederberg (biologist, Nobel Prize in Medicine 1958), Lubert Stryer (biochemist, National Medal of Science 2007) and Avram Goldstein (MD but also pharmacologist). Stryer took a sabbatical in order to head the research team at Affymax.

It was Goldstein who argued that it should be possible to take the example from immunology where a rather limited number of peptide molecules produced by the body can be combined into an enormous number of different antibodies that can recognize (i.e. bind to) any intruder molecule (antigen). Michael Pirrung (a chemist) and Leighton Read came up with the idea to apply a production method used in the semiconductor industry in near-by Silicon Valley to the *in situ* peptide synthesis: a photolithographic, or light-directed technique. Fabian Pease, a professor at Stanford specializing in the development of electronic chips, joined the team (Lenoir & Giannella, 2006).

Stephen Fodor came to Affymax in 1989. His career progression is emblematic for the relationship between biology and chemistry: Bsc in biology, a Master's in biochemistry and a PhD in chemistry. He insisted on using the photolithographic technique developed also for the *in situ*

synthesis of DNA microarrays and published his results in 1991 (Fodor *et al.*, 1991). He founded the company Affymetrix to exploit his invention and bring the DNA Gene Chip to the market. However, the technique developed by Fodor is partly covered by patents held by Southern, who successfully sued Affymetrix for copyright infringement (the interested reader is referred to the article by Rouse and Hardiman on the history of industrial property in the microarray domain (Rouse & Hardiman, 2003).

### 5.1.3. The Seattle Group

Edwin Southern was the first to suggest the use of ink-jet printer heads for the *in situ* synthesis of DNA.

Alan Blanchard (a mathematician) went on to explore this idea from the early 1990s onwards at the California Institute of Technology. He worked alongside Leroy Hood (MD, he received the *Albert Lasker Award for Basic Medical Research* in 1987), following him to Seattle when the latter set up the Department of Molecular Biotechnology in 1992. They teamed up with the heads at the Fred Hutchinson Cancer Research Center, Leland H. Hartwell (*Albert Lasker Award for Basic Medical Research* 1998, Nobel Prize in Medicine in 2001) and Stephen Friend.

Blanchard perfected the use of ink-jet printer heads for the *in situ* synthesis of DNA when working at Rosetta Inpharmatics Inc., a company set up by Friend in 1997. The patents for this technology went to Agilent Technologies, a former daughter company of Hewlett-Packard (which was not only in the printer business but also specialized in instruments and kits used in molecular biology) at the end of the 1990s. The project drew staff with very different backgrounds, from a variety of HP departments (ink jet printers, scanners, software, micro-fluidics and chromatographic equipment) as well as academia.

Agilent Technology developed a microarray, which is produced on an industrial scale and which competes with Affymetrix's Gene Chip on the market for *in situ* manufactured microarrays.

## 6. An Open Source approach: The Institute for System Biology

The three examples described above are all commercially orientated; the labs buy the ready-to-use product.

The *in situ* synthesis of DNA using ink-jet printer heads is, however, a technique that can be carried out using quite basic material, within (economic) reach of a biology lab. The Institute for System Biology, a

non-profit organisation created by Leroy Hood, publishes all the information necessary “Open Source”.

Interestingly, J. Leighton Read, one of the founders of Affymax is on its board of directors (Lausted *et al.*, 2004).

## 7. Spotted Microarrays

Microarrays using the *in situ* synthesis of DNA are mainly used for organisms that are widely studied, like man and mouse. Biologists also have the possibility to use microarrays where the completed oligonucleotide is deposited on a nylon or glass surface, the so-called spotted microarrays.

As it is a generalization of the Southern blot, this technique is a rather natural and obvious choice for biologists. They first proceed as described in “Some typical working methods in biology”; then a robot will deposit the DNA fragments on the chosen surface (nylon or glass). The DNA fragments have been obtained from genomic libraries (see insert). The necessary equipment is available on most campuses as it is relatively inexpensive. On the other hand, it is a method that is highly labour intensive and the results are not as reproducible as with the *in situ* synthesis.

The technique was developed at Stanford in 1992-94 by Pat O. Brown (a chemist who received a PhD in biochemistry before becoming a medical doctor) and Dari Shalon (an engineer) (Schena *et al.*, 1995; Brown, 2009).

It is freely available for non-profit use and the inventors describe the protocols and equipment necessary on the Stanford Microarray Database website. This has not kept them from also creating a society that commercializes ready-to-use spotted microarrays.

## 8. Some Concluding Remarks

### 8.1. The Ties between Chemistry and Molecular Biology

There is no clearly defined boundary between biology and chemistry in molecular biology, even if industry prefers using techniques from the world of chemistry (for example the *in situ* synthesis of DNA) as they are less labour intensive.

The scientists in this field have often moved from one discipline to the other during their careers. The key techniques were invented by biologists, chemists, physicists or teams combining different know-hows; one cannot clearly distinguish a relationship between the initial training of the

scientists and the (research) field one would be inclined to attribute their inventions to.

The technological environment, on the other hand, does play a crucial role (Southern worked at a university which produced a considerable amount of the tools used in molecular biology, Affymax had its location in Silicon Valley and favoured the techniques used in micro-electronics, Agilent exploited the know-how of Hewlett-Packard).

The most important factor, though, is probably the dynamism of a group of creative scientists who come from different scientific fields, clearly exemplified by the teams at Edinburgh University, Affymax and Agilent. These teams or constellations can only exist as long as their research does not become part of the Establishment: the barriers of each discipline will then be drawn up again.

## **8.2. DNA Microarrays: A Revolution in Midstream**

The aim of all the techniques described in this chapter is to measure the concentration of a molecule, which does not possess any easily measurable physical-chemical properties and which is present in only very small quantities in a biological sample. The most original aspect of the microarrays is that they describe each sample with tens thousands of quantitative data. This in turn creates a new problem: how can one draw a maximum of information from this mass of data?

Analysing quantitative data is nothing new in biology (take the example of the variance used in plant breeding or the discriminative analysis used in medical diagnostics) or in chemistry (for example partial least square regression (PLS) used in formulation chemistry), but until now scientists worked on only a small number of data, a few dozens at most, using statistical tools often dating back to the first half of the 20th century. The most important lesson to be remembered is that the data cannot be fully exploited unless all the factors involved in the experiment are combined in a rational manner (as in the experimental design drawn up by Ronald A. Fischer in the 1920s) (Riva *et al.*, 2005).

Experimental design is not part of the methodological heritage of a molecular biologist. Indeed, an entire branch of molecular biology, genetics, was built up in opposition to biometrics and to a holistic approach (note that in biometrics a gene is a statistical concept, a correlation between the values of a characteristic measured in the parents and their offspring, and not a molecular entity). The geneticists have therefore developed a reductionist's experimental approach: one isolates a single factor and equalizes everything else. This explains why nowadays

the majority of analyses using microarrays are carried out picking out a small amount of data. The biologist already possesses some knowledge on them; the measurements are replaced by quasi-qualitative evaluations (“varies little or a lot”).

Introducing the concept of experimental design in molecular biology is a necessary step forward, although most probably not a sufficient one. Specialists believe that the optimal exploitation of the enormous quantity of data generated by microarrays remains an open problem.

Mathematicians and linguists are joining forces with biologists and chemists in an effort to solve this problem (as exemplified by Sage Bionetworks surrounding the Seattle group (<http://sagebase.org>)).

So far, however, we do not observe any interdisciplinary careers as have woven through the history of the relations between chemistry and molecular biology. It would be interesting to know why: is there a lack of multidisciplinary in the original training? Are the reasoning methods too different? Must we look for other reasons? An epistemological investigation of these questions would also help to understand the ease with which the relations establish themselves between chemistry and molecular biology.

## **9. Insert: How to build a Genomic Library (A Simplified Account)**

### **9.1. The Reason for Describing this Procedure**

It is a procedure carried out in a wide range of biology labs. The various steps in this quite laborious procedure show rather well the mixture of chemistry and biology based techniques typical of a biologist's work in the wet lab. It is also a necessary step for the preparation of spotted microarrays.

### **9.2. What is a Genomic Library?**

It is a collection of bacterial (or yeast) colonies where each colony contains a fragment of another organism's genome, the organism one wishes to study. Taken together, these fragments make up the entire genome, i.e. contain all the genetic information of that organism.

### **9.3. Why Build a Genomic Library?**

There are basically two reasons: first, the researcher might want to sequence the organism's genome, in other words identify the nucleotide

sequence of the DNA molecule(s) contained in the organism. Second, the researcher might want to study a particular gene (or several) of that organism.

In both cases the researcher needs a large number of copies of the genetic material. If it is problematic to obtain the necessary amount of DNA of the organism, for example because it is difficult to grow in the lab, it makes sense to transfer pieces of the organism's DNA into an organism that is easy to grow and that will produce large quantities of the DNA required in a reproducible manner over a long period of time.

The procedure illustrates nicely a fundamental approach in biology: modifying a living organism to make it produce a desired macromolecule in the quantities needed.

#### 9.4. How to Proceed

1. Isolate a sample of DNA from the organism's cells: DNA extraction  
The material containing the DNA is washed with detergents removing any non-DNA molecules (like lipids and proteins). The DNA is precipitated by using alcohol and can then be extracted by spooling it onto a glass rod. The DNA is stored in a suitable solution at low temperatures until further use.  
This is a chemistry-based step.
2. Cut the DNA into large fragments  
The DNA is cut into large fragments (a few thousand nucleotides or more) using a restriction enzyme. Nowadays a huge number of these enzymes is available in the lab. Each enzyme cuts the DNA at an idiosyncratic nucleotide sequence.  
This is a biochemistry-based step.
3. Cut a cloning plasmid with the same restriction enzyme  
A cloning plasmid is a small, circular molecule of DNA that can be easily inserted into the host organism (the bacterium) used to build the bank. The cloning plasmid is a biologist-made genetic construct, which possesses several important features: a gene conferring antibiotic resistance (e.g. to ampicillin), a gene for producing the enzyme beta-galactosidase and restriction sites for several restriction enzymes situated within the galactosidase gene. It is easy to highlight the activity of the enzyme beta-galactosidase using a colorimetric test: the bacterial colony will turn from white to blue in the presence of 5-bromo-4-chloro-3-indolyl-beta-D-

galactopyranoside (or X-gal in the biologist's jargon) when the enzyme is active.

The plasmid is opened with the same restriction enzyme used in the previous step, cutting the beta-galactosidase gene.

The creation of a cloning plasmid falls into the domain of biology, its opening using a restriction enzyme into that of biochemistry.

4. Fusion of the DNA fragments and the cloning plasmid

Mix in one test tube the cut genomic DNA (the fragments), a high concentration of the cut plasmids and DNA ligase. The latter is an enzyme that joins cut pieces of DNA together.

Under the influence of the ligase some plasmids will simply close again, but others will have taken up a fragment of the foreign DNA. These are called recombinant plasmids.

The test tube now contains a mixture of plasmids: recombinant and not.

This is a biochemistry-based step.

5. Incorporate the plasmids into the bacterium used for the construction of the library

Add the plasmids to a bacterial culture that is susceptible to an antibiotic (in our example ampicillin) and does not possess the gene for beta-galactosidase. The cells may have to be briefly warmed and given a small electro-shock in order to take up the plasmids. The details of the protocol to follow depend on the bacterial species used.

This step falls into the domain of biology for two reasons: 1) It is necessary to work under sterile conditions to avoid a contamination of the bacterial culture through other organisms; 2) the biologist has the necessary expertise to develop a protocol which allows an efficient take up of the plasmids.

6. Plate the bacteria on plates containing ampicillin and X-gal

This entire step has to be carried out under sterile conditions, following rules that have been observed in microbiological labs ever since Pasteur.

The bacterial culture is plated on to Petri dishes containing a growth medium with ampicillin and X-gal. The bacteria, which did not take up a plasmid, will be killed by the ampicillin. Bacteria, which have taken up a plasmid are antibiotic resistant and can grow. Those who have taken up a non-recombinant plasmid will break up the X-gal with their beta-galactosidase, forming blue

colonies. Recombinant bacteria no longer possess an intact gene for beta-galactosidase, as a fragment of the foreign DNA has been integrated. These bacteria will form white colonies and are those of interest to the researcher.

The biologist will now take each colony one-by-one and purify it in order to make sure that each colony has been formed by a single bacterium.

Each colony will contain one DNA fragment of interest, forming one element of the genomic library.

Again, this step falls into the domain of biology for two reasons: 1) it is necessary to work under sterile conditions; 2) the reasoning behind the selection procedure for the colonies is typical for geneticists.

7. Make a large collection of white colonies to form the genomic library.

The incorporation of DNA fragments into plasmids and the selection of white colonies are processes dictated by chance. To make sure that each fragment of genomic DNA is contained in at least one bacterial colony, the researcher has to have 8 to 10 times more colonies than DNA fragments: if the organism's DNA was cut up into 1000 pieces, he will need to make 8 to 10000 colonies, the genomic library.

If the purpose of the genomic library is to sequence the genome of the organism, the researcher will create two libraries (each with 8 to 10 000 colonies) using two different restriction enzymes, which cut the DNA at different sites of the genome. That way he obtains DNA fragments that overlap, allowing him to reconstruct the order in which the fragments make up the complete genome.

This is rather typical for biology: despite all the ruses used and regardless of the amount of resourcefulness applied, the experiments are long and highly labour-intensive.

## 9.5. How to Select a Particular Gene

If the researcher is interested in one particular gene, he has to find the one colony amongst the 10000, which contains this gene. He will have to know at least some property of the gene or the protein it codes for, which will allow him to construct a probe, following one of the methods described in the section "The concept of molecular marking".



The researcher will choose a biological or biochemical approach according to his tastes and the nature of the task. Given enough time and effort, he will eventually find the needle (gene) in the haystack (the genomic library).

Once the colony of interest identified it can be easily grown, thus also multiplying the plasmid containing the desired gene. The plasmids are then harvested and the gene (or its product) extracted.

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# CHEMISTRY AND INTERFACES

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## Introduction

This collective work explores the role of interfaces within the different domains of chemistry. It deals with the interfaces between solids, liquids, and gas but also those between science and technology, academic and industrial research, and between various specialties (physics, biology, material sciences, nanotechnology, and so on). Our starting point is the chemical practices themselves. In line with Denis Diderot (1754) and the later Wittgenstein, we agree that a careful study of what people actually do within the “terrain” of their activities is of importance and should be addressed by considering their specific sites, devices, instruments, and goals. Our main aim is to scrutinize the importance of such interfaces in order to provide philosophers with new ways of thinking about the scientific community, paradigms, scientific innovation, science and technology.

## 1. Interfaces in Solutions and in Chemistry Itself

Let us start by the description of an interface described by Stéphane Sarraide, a French leading specialist of extraction by means of supercritical carbon dioxide at the CEA (Center of Atomic Energy). He will also analyze his own experience concerning his current interactions with other specialists from different domains.

The fundamental states are the chemical phases in which a material balance exists in its immediate environment. These different states are located in a phase diagram, a map of the given material as a function of temperature and pressure. Pure substances (water, carbon dioxide, oxygen or nitrogen) can typically exist in solid, liquid or gaseous form, or even

plasma, which is less trivial. We learned in school that a walk on this map, the phase diagram, costs energy. Indeed, moving from one state to another, for example from liquid to gas, requires crossing a boundary of the phase diagram: the liquid / gas interface. At constant pressure, the energy can be given by heating the liquid; part of this energy is used to make the material passes through a discontinuity: this is enthalpy change, called heat of vaporization in our example. Historically also known as “latent heat of state change”, this energy is not lost but is latent, which is to say, hidden somewhere in the interface. So, could the chemical interface be a discontinuity synonymous with energy?

Certainly, and some discontinuities are located in singular points within the phase diagram. To identify them, imagine a water bottle half empty, or half full if we are optimistic. It is a container filled with a liquid phase in equilibrium with its gaseous headspace (vapor), in the middle a visible interfacial zone. In this simple system, we walk in the phase diagram, increasing the pressure and temperature. Arrived at a particular point of the diagram, the critical point, the interface disappears and the two phases (liquid and gas) disappeared in favor of one: the supercritical phase. Beyond 221 Bar and 374 °C - the coordinates of its critical point, water will be in supercritical phase, with properties of both liquid and gaseous states. Please note that the supercritical phase is not a fundamental state of matter, rather it is a homogeneous and stable phase, at the limit of instability.

Let's go back to the critical point, a very singular discontinuity. It corresponds, in the phase diagram, to the specific point where the interface is broken, and where the energy is thus theoretically released. It is quite the case because if we measure the physical properties of water at this point (specific heat, conductivity, compressibility, etc.), they would be equal to 0 or infinity as non-analytical values. So the critical point of pure compounds might be regarded as a kind of black hole, which enables chemists to become aware of the huge quantity of energy concealed in an interface.

Interface can also be regarded as a boundary between two immiscible liquids placed in a container. These two chemically incompatible liquids will generate a minimum surface exchange, organized in a plane under the action of gravity. Geometries of different interfaces are conceivable in the absence or with modifications of gravity. An interface results from the minimization of the contact between two immiscible “geometric entities” and is thus a particular place that allows transfers. In a given liquid, the physicochemical properties are duplicated continuously at the walls of the container and especially at the interfacial zone. The molecular organization

of this area implies that the thickness of an interface is zero. Indeed, the conceptual view of an interface may be seen as a plane positioned between two half-interfaces made of the two immiscible liquids. Between the two half-interfaces is found what we can call “the interface”, a mathematical plane of zero thickness. All of this constitutes the interfacial zone that is macroscopically visible.

To sum-up, this kind of interface is conceptualized as a boundary of zero thickness, full of energy and allowing transfers between two separated liquid species. Could it be the same for knowledge?

In a chemistry laboratory, researchers are constantly interacting. Research is a cooperative adventure, multiplying the areas of contact between researchers: interfacial areas. An experimenter wishing to carry out a chemical reaction will have to generate multiple exchanges. The first collaborators will be some thermodynamicists who will investigate and assess the theoretical possibility of the chemical reaction from the outset. Chemical engineers will then imagine the experimental process by determining all the operational conditions (pressure, temperature, etc.). Finally, theoretical modelers, be they specialists in quantum chemistry or in molecular dynamics, will try to understand the basic mechanisms of this reaction by means of suitable equations sets displayed on a computer screen. In current chemistry, the interface between modelers and experimentalists is a fine line around which iterative constant exchanges revolve in order to generate knowledge. Robust chemical models, those that faithfully reproduce the experiment, can be pushed to their limits. Indeed, it is possible to extend the operating conditions at the entrance of a robust model for providing new areas of operation. This practice is called “simulation”. Simulation allows chemists to create new interfaces with engineers in order to scale-up the process from laboratory to industry.

So, in a chemical laboratory, interfaces are needed between the various researchers to develop knowledge. These are the exchanges between the different “entities” that generate the energy of knowledge.

When my research team and I developed the concept of “cork stoppers” treated with supercritical CO<sub>2</sub> and guaranteed free of cork taint, we had to create many interfaces in order to reach this goal. In that time, I was the head of the laboratory. In doing such a job, I found myself at the very initial interface between the industrial partners and my research unit. The specifications were drawn; the goal was to remove trichloroanisole from cork, the natural molecule responsible for cork bad taste in wines, even at very low concentrations. Thermodynamicists studied the solubility of the molecule in supercritical CO<sub>2</sub>. Analytical chemists then developed methodologies to analyze samples before and after treatment in order to

assess its effectiveness. Laboratory technicians proposed skilled improvements so as to determine experimentally at what operating conditions the extraction could take place. Finally, the chemical engineers addressed industrial extraction by estimating actual returns. In doing so, they validated the technical and economic relevance of the whole process. After 7 years of research, an industrial plant of 800 million caps per year treatment capacity was established, the result of an incalculable amount of interfaces. And what about the new fields of knowledge in modern chemistry?

They can be seen in the same way. It is conventional to assume that physics is primarily concerned with elements smaller than atoms whereas chemistry starts above the atoms, from the ions and molecules. The atom can therefore be considered as an interface between these two disciplines, and exchanges arising from them will produce new knowledge such as quantum chemistry or atomistic simulation.

In the same spirit, pure chemistry ends when the chemical agents to study become numerous and organized with each other. In this context, we gradually enter into the realm of biology. As before, the interface between chemists and biologists has opened new horizons, those of biochemistry, biotechnology and, closer to us, the pharmacy of the future. The new therapeutic approaches are based on interactions between chemists and biologists; this is the case of gene therapies and new therapeutic targets. Alessandra Gucki Riva, Alain Hénaut and Daniel Daugeron query the interface between chemistry and biology within this part of the present volume. They scrutinize how their interactions gave rise to the microarrays technology.

I was confronted with this approach of creating an interface between chemistry and biology within the framework of a common program developed between a French pharmaceutical company and my laboratory. The idea was that molecules of active pharmaceutical ingredient (API) are often poorly soluble in conventional solvents such as water. The trouble is that our body consists of approximately 70% water which leads pharmacists to on-dose API, often expressed in drugs mg, in order to statistically increase the amount of drug in the treatment area after ingestion. The idea was to solubilize the API in supercritical CO<sub>2</sub> under a sudden drop of several hundred bar pressure. The active pharmaceutical ingredient was micronized and then became much more soluble in the human body. From the perspective of chemists, we have studied the solubility of an active pharmaceutical ingredient in supercritical CO<sub>2</sub> and then we characterized the micronized aggregate. Creating an interface with the biologists was the initial step, because it was essential to determine

whether the molecule roughly treated by chemists kept its polymorphism, that is to say, its structural integrity, directly related to its effectiveness. Once done, it was then time to talk to the pharmacists who were tested new API on guinea pigs in order to check the effectiveness of micronized molecules. Finally engineers specializing in the pharmaceutical industry joined us so as to translate our laboratory process into an industrial one in compliance with the international standards of the good manufacturing practices of pharmaceutical industry. I still bear in mind these multiple interfaces created between theoretical chemists, biologists, experimentalists, and chemical engineers. In a way, it was like entering into an unlikely scientific tower of Babel. We therefore had to manage multiple interfaces so that concepts could spread despite the hyper specialized vocabularies of our disciplines. Finally, the method allows obtaining with just 1 mg of micronized molecule the same therapeutic effect than that obtained with 1000 mg of initial API. This is the result of immense energy used to make the interfaces between our different scientists' worlds permeable.

The interface is thus at the heart of the chemical processes. Up to a certain point, it can even be regarded as a root for the future of knowledge in this discipline, and more generally for science. In line with us, other contributors of the present volume such as Sylvain Caillol on the one hand, and Laura Maxim and Isabelle Rico-Lattes on the other, have respectively shown how interfaces between specialties are at stake in the development of sustainable chemistry. As the philosopher Joseph Rouse asserts: 'What results is not a systematic unification of the achievements of different scientific disciplines but a complex and partial overlap and interaction among the ways those disciplines develop over time' (Rouse, 1996, p. 177).

We will further develop this perspective in the following paragraphs. Let us now illustrate the importance of interfaces in materials chemistry, a growing field today.

## **2. Chemical Materials: A Crossroads of Practices**

Let us first study how chemists create, analyze, and use materials in various fields in order to achieve new specific goals.



## 2.1. A Classification of Materials

### a. Chemical Bonding at the Interface between Two Atoms

The notion of classification leads chemists instinctively to the periodic table of Mendeleev, which provides a systematic classification of the chemical elements. From the material chemists' point of view, it is generally accepted to establish a ranking of "solids" based on the nature of the chemical bonds present in the material. Always questionable, this classification is used to group most of the materials. The characteristics of resulting atomic and structural properties distinguish three broad classes of materials: metals, organic polymers, and ceramics. The combination of two materials from these different "families" gives rise to a fourth class of materials, namely, the composites. Below is a diagram showing the different classes of materials.

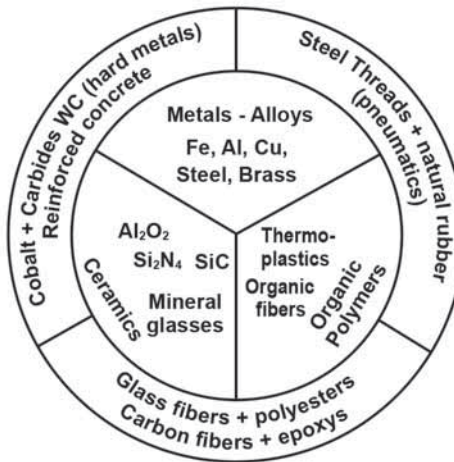


Figure 1: Different classes of materials (Mercier *et al.*, 1999).

Metals constitute most of the periodic table elements, including the transition metals (copper, iron, zinc, etc.), alkali metals (sodium, potassium, etc.), and alkaline (magnesium, calcium, and so on). The source of metals properties such as their electronic or thermal conduction, and opacity to visible wavelengths can mainly be explained by the metallic bond. From a mechanical point of view, metals are plastically deformable, tough (high resistance to cracking), and have high melting temperatures.

The combination of a large number of molecules of low molecular weight named monomers gives birth to the organic polymers. A new

macroscopic molecule or macromolecule of high molecular weight is obtained. The polymer can be seen as a chain of carbon atoms, more or less ramified (two-dimensional or three-dimensional) containing oxygen atoms, hydrogen or chlorine for example. The chemical reactions used to create these materials are called polymerization reactions (radical polymerization, step-growth polymerization, etc.) and give essentially rise to covalent bonds within the network. These reactions are usually associated with organic chemistry and not with solid-state chemistry because they use organic molecules from the outset. However, these materials are an essential part of material science because of their lightness, thermoplastic and shaping properties at low temperature and for a very low cost.

Ceramics are the last family of materials. The first clay-based ceramics were certainly discovered shortly after the discovery of fire, which makes this class the oldest. Ceramics can be defined as non-organic materials and non-metal consolidated at high temperature. They are usually the result of the reaction between one or more metal atoms (Al, Mg, Fe, etc.) with a non-metallic compound (oxygen, nitrogen, carbon, etc.) at high temperature. Ceramics are known for their excellent heat resistance (refractory ceramic). They are also known for their hardness and that is why they are often used as abrasives. The term ceramics applies to both ceramic compounds described above and to inorganic glasses or cements. In all cases, the materials are characterized by the presence of covalent and ionic bonds.

The chemical bond is one of the essential criteria in this classification. In all the materials, it is precisely the chemical bond that allows cohesion of atoms. The metallic, ionic or covalent bonds dictate most of the material's properties. The electronic characteristics of the atoms will determine the nature of the connection and thus the interface between these two atoms. It is through this *interface* that the three types of materials described above were classified. The last class of materials to be presented is a separate category. It results from the combination of two or more materials that belong to the families described above. In this case, the resulting properties are no longer strictly related to the bond between two atoms, but more generally to the interface between both materials.

## **b. Composite Materials**

As seen before, each family has different properties (ductile and tough metals, soft and light polymers, refractory and high tensile strength ceramics). The combination of two immiscible materials can be used to

create new materials: the composites. Their properties may have resulting properties that combine the advantages of both materials but not systematically. For example, in aviation it is highly appreciated to lighten the structures while maintaining excellent mechanical strength. It is generally difficult to say that the resulting properties of the composite are equal to the sum of material properties taken separately. Indeed, the combination of two different types of materials will generate an interface between these two elements. In this respect, interfaces are crucial regarding what some philosophers call *emergent* or *resultant* properties. Novelty is not solely a matter of basic ingredients or laws (taken in isolation or in interrelation) but also a problem of interfacial dynamics.

In the field of civil engineering, reinforced concrete is a well-known composite material that is extensively used. It resulted from the combination of concrete (ceramic) with steel rods (metallic material). The concrete has a high compressive strength but poor tensile strength. To overcome this drawback, the idea of incorporating steel rods that have both excellent compressive and tensile strength resistance leads to a composite material that resists both tensile strength and compression. In this example, as in most composite materials, the notion of interface is a very important one. In a composite material, the components are immiscible and therefore, an interface is created, the properties of which must be fully investigated. Differences in chemical or physical reactivity of each of the components induce changes at the interface that can destroy the properties of the whole composite. In the case of reinforced concrete, corrosion of steel rods induced by the water contained inherently by the concrete induces changes at the steel / concrete interface and may result in an early termination (Dorlot *et al.*, 2002).

### **c. Material as a Solid Object**

A distinction may be already pointed out, that is to say the tendency to see materials only as solid “objects”. Neither liquids nor gases are present in the families described above. In the 1950’s, material chemistry was called “Solid state chemistry”. The solid state in the physical sense was studied, whether in metallurgy or inorganic chemistry for example. The industrial context is more and more prominent in laboratory so that research has gradually transformed the term “solid state chemistry” into that of “materials chemistry”. This semantic shift partly results from interactions at the interface between academic and industrial researches. Scientific changes (conceptual, taxonomic, and instrumental, among other aspects) are often matters of such interfacial transformations.

The solid state is the common point of the different classes of materials. The transition from solid to liquid state is generally related to an increase of temperature or pressure. The materials are therefore considered to be solid at the temperature and pressure they are used. From a thermodynamic point of view, any solid may become liquid by raising the temperature. However it will lose the chemical and physical properties that make it unique for an application. But there exists some materials on the borderline between the solid and liquid state. In a glass for example, the solid definition is not as strict as it seems. A glass is by definition a congeal liquid. Therefore, it could be considered as “solid-liquid”.

The liquid state has very specific properties, it has a viscosity, it is possible to sink it and the liquid can take the form of its container. The solid state has other specific properties; it can break, may have defects in its structure, and so on. The manufacturing of glass from a liquid to its final solid state is quite apart in material chemistry. It has both features of the solid (presence of defects, it can break under mechanical stress) and liquid properties as well (viscosity, structure, etc.). The glass is somehow at the interface between the solid and liquid, and most of its properties are related to this interface. Some chemical materials have in-between properties that put under questions classical frontiers between solids, liquids, and gas. Chemists often upset usual taxonomies by creating new materials or chemical bodies that intertwine alleged incompatible characterizations.

## 2.2. The Glass: Between Liquid and Solid

Glass is often defined as a non-crystalline solid that displays a glass transition (Zarzycki, 1997). The glass transition temperature is the temperature under which the glass is transformed from a solid glassy state (solid) to a solid-plastic (viscoplastic state). A glass is obtained by quenching a liquid from high to a lower temperature. A liquid mixture at high temperature is quickly cooled down to the solid state by a thermal quench. Hence, it has a physical solid state, but considering the atomic scale, the structure is close to the liquid from which it is originated. Solids such as metals, ceramics, or crystals are ordered; scientists usually speak of long-range order. The atoms are placed with precise coordinates in an elementary volume that is repeated endlessly in all three spatial directions. The glass is completely different; it is usually called a *disordered solid*. The unique optical and thermoplastic properties are directly linked with this structure.

The glass is a material that is out of the thermodynamic equilibrium. During the synthesis of a glass the liquid is forced to become a solid, which means that it actually keeps its structure in the atomic scale. Therefore, it can be considered as an unstable material. One of the major interests of the glass is its structure between the liquid and solid. Below the glass transition temperature, the glass is in a solid form (“infinite” viscosity). When it is heated above this temperature, the glass passes through an intermediate state between solid and liquid state called “viscoplastic” or “plastic-solid”. The glass becomes less and less viscous. In this physical state it is possible to draw it under optical fiber or mold it in the desired shape for optical lenses for example. The glass transition is a reversible phenomenon. By decreasing the temperature to room temperature, it is possible to get the glass in its physical solid state (Haussone, 2005).

Obviously, there are limits to this unstable state. After a certain temperature, the thermal energy provided will be large enough to allow the atoms to rearrange. In other words, the glass that had a short-range order rearranges. As a consequence, lengths and angles of chemical bonds change gradually to return to their thermodynamic equilibrium. This stable solid is the crystal that has the lowest energy. From this temperature (crystallization temperature) properties change drastically, the material gradually loses its viscoplastic properties, transparency and all of its physicochemical properties (thermal conductivity, electronic density, etc.).

The solid and liquid states are closely linked in the example of a glass. This interface between liquid and solid that looks so clear is somehow blurred when we consider the particular case of the glass. In this material these two states *coexist*. The interface between liquid and solid can be seen as the glass transition itself. Below this temperature the glass has an “infinite” viscosity, and therefore it can be considered as a solid. Beyond this temperature, the glass recovers the characteristics of the liquid that gave rise to it. This phenomenon is endothermic and reversible, so it is theoretically possible to switch from one to the other of these two states indefinitely as long as no crystallization is observed. The characterizations of glass thus depend on the context and on the device within which they are *afforded*. We use the verb *to afford* in line with the definition proposed by Rom Harré in the third part of the present volume in order to insist on the role of the interactions and the operations in the very definition of a chemical body. This context-sensitiveness is of importance for chemical ontology insofar as its queries what philosophers call chemical “individuals”.

As we have seen, the optical properties of glass and thermoplastics are particularly interesting, but the material chemistry is also linked to an application. Application is the aim of a lot of objects that human beings have created. A fragile glass will not be useful in extreme conditions of pressure and temperature. But a glass will be taking advantage from its transparency in the visible and chemical resistance to the external environment; hence it is used for the windows or in a car as the windscreen. This transparency allows us to see the outside world from the inside. Because of its specific structure between the solid and liquid states, it acts also as an “invisible” interface between the outside and the inside of a building! The strength of particular materials depends on their applications, and conversely, the strength of an application will be linked to the quality of the particular materials.

### 2.3. From Synthesis to Applications

The chemist's role in the production of a material is undoubtedly the synthesis. Indeed, during the chemist's scholarly background, she had the opportunity to learn different methods of synthesis for different compounds (metallurgy, ceramics, and so on). She is probably more able to ask critical questions related to the synthesis (purity, defects, method of synthesis, devices, etc.) and to answer these questions by means of experimentation.

However, the idea of designing or studying a material can arise in different ways. The interest of a material chemist may be stirred up if she envisages a combination of atoms or molecules that have never been combined so far. She will then investigate the resulting properties of this new association. The idea of a material can also be motivated by an industrial need. When a potential market is identified, or if a material that already exists needs to be improved (better resistance or lower cost for example) the manufacturer will use material chemistry to determine how he can possibly replace or improve the existing material. Finally, a material can be created by chance from an uncontrolled experiment. In this respect, the material is considered to be an intriguing compound that needs to be further investigated.

In each case, the knowledge of the physical and chemical properties follows the synthesis of a material. This property may be electrical, semiconducting, magnetic, mechanical, chemical, optical, etc. It is generally linked to the electronic or atomic structure. The nature of chemical bonds, physical shape (phases, grain size and particle shape, surface state, presence of defects, etc.) is a clue to understand the material's properties. If one bears those considerations in mind, the case of

a glass ceramic becomes pretty interesting. A glass is inherently brittle and fragile. It is well known that the generation of small crystals in large quantities improves the mechanical properties while maintaining the transparency of the initial glass. In this case, it is precisely the interface between the crystal and the glass that improves the toughness. When a crack propagates inside the glass and meets a crystal, its potential energy will decrease drastically. In this example, we clearly see that the role of the chemist is not only dedicated to the synthesis. If she wants to fully understand what is going on through the material under mechanical stress for example, she must discuss and interact with scientists from other disciplines in order to provide a scientific explanation.

In the Great Pyramid that leads the material from conception to market, chemistry can be seen as the base of the pyramid. But in every scientific field (mechanics, optics, physics, and so forth) and industry, academic researchers work together. Each step that is climbed resulted from interactions between all those fields. It should be pointed out that different areas will be constantly working together and reconfiguring their initial views in order to get an interesting material for a specific application.

To illustrate the relationship between academic and industrial research, let us take the last example of the making of a glass-ceramic for application in a night vision goggle. The use of glass-ceramic is motivated by the need of improving mechanical properties of glasses. Indeed, the weak point of glasses is their poor thermo-mechanical properties that weaken the equipment and restrict their applications. A lens is roughly composed of a glass and antireflective coatings used in order to get rid of losses by reflection. The market and the field experience of the industrialist render her unable to identify the inherent limitations of the material. That is to say, they know what to improve and to maintain. Once needs are identified, private or/and public agencies investigate possible ways to replace or to improve the product. For example, the chemist can work on the choice of glass, its purification, among other parameters. A change in composition can improve some of the properties, or even can lower the cost. However the new properties of this glass or glass-ceramic will induce changes in the deposition parameters of antireflective coatings already optimized by industrial researchers (thicknesses of layers interface between the glass coatings). To reach the customer and industrial expectations, industry and academy have to work together in order to reach their goals. If the common goal of the chemist, the engineer and the optician is to get a commercially viable product at the end of the chain, it is imperative that they put in common their knowledge and expertise. All areas are connected to a material and its application from the outset.

Collaboration and emulation among chemists, physicists, engineers, and opticians are necessary to obtain a material corresponding to the desired criteria. To sum-up, the interface between all the scientific fields in materials science is of paramount importance to carry out the production of the new material (Rozé *et al.*, 2011). Let us now further explore the role of interfaces during the synthesis of a material.

## 2.4. Interfaces and Soft Chemistry: The Case of the Precipitation Process

If ceramics are traditionally prepared from natural resources, the development of technical ceramics and the progress in nanotechnologies has dramatically increased the demand for precursors of higher purity and with better controlled compositions and sizes. The synthesis of ceramic powders by precipitation is popular because it is a simple process, and is often called “soft chemistry” or “chimie douce”, to describe processes working at low temperatures and pressures in an aqueous environment (Jolivet *et al.*, 1994). In this type of synthesis the *solid/liquid interface* is at the heart of the whole mechanism.

### a. The Different Steps of Precipitation

Precipitation involves a phase change, where solid particles are created from a liquid phase with sizes and morphologies depending on the operating conditions (Dirksen & Ring, 1991; Söhnel & Garside, 1992; Haussonne *et al.*, 2005; Myerson, 2005). The thermodynamic driving force for the formation of the new phase is the saturation ratio  $S_R$ , which is given by  $S_R = C_l/C_s$ , where  $C_l$  is the solute concentration and  $C_s$  is the equilibrium solubility at the temperature and the pressure of the system. The overall free energy  $\Delta G$  is the sum of the free energy corresponding to the creation of a new volume and new surfaces (Eq.1):

$$\Delta G = - \frac{V}{v} k_B T \ln(S_R) + \gamma A \quad \text{Eq.1}$$

where  $V$  is the volume and  $A$  the surface of the new aggregate,  $v$  is the volume of the embryo, and  $\gamma$  is the surface free energy per unit area. Spontaneous precipitation is observed when  $S_R > 1$ . In these conditions,  $\Delta G$  has a positive maximum at a critical size  $r^*$ .

When precipitation occurs, the first step corresponds to the creation of new stable solid surfaces, and is called *nucleation*. This is the most important step, where molecular species, called “embryos” are created.



Their number and their nature will determine the final properties of the material. This is however the most difficult step to study, because of its rapid kinetics, the instability of embryos and their small sizes.

The nucleation process can be broken down into three main categories. *Homogeneous nucleation* occurs in a homogeneous medium, free of impurities and solid interfaces. These conditions are scarce, and it is actually very difficult to avoid dust, interactions with the reactor walls, or surface heterogeneities. In practice *heterogeneous nucleation* is most likely observed, because nucleation on a foreign surface is favored by a lower surface energy. Some fine particles of the precipitate can be introduced into the reactor in order to ensure a better control of nucleation by “seeding”. Finally *secondary nucleation* can occur when growing particles collide with the walls of the reactor, the stirrer, or other particles, breaking off fragments that become seeds.

Nucleation is followed by the *growth* step. When seeds become larger than the critical size they will further decrease their free energy through the addition of molecular species or growth units. At low saturation ratios, nucleation and growth are slow, and monocrystalline growth is favored. The crystal equilibrium shape is obtained with very slow kinetics. Other morphologies are observed, depending on the supersaturation and the growth mechanism: layer-by-layer, mononuclear, polynuclear, screw dislocation, and so on. Finally polycrystalline structures are obtained through an agglomeration process, leading mostly to spheres (Figure 2).

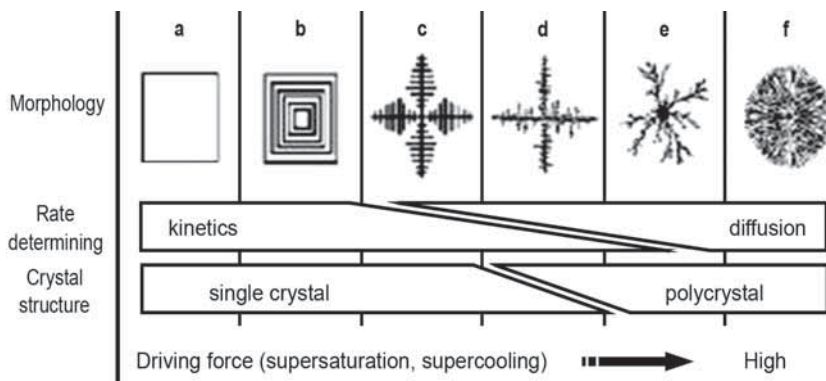


Figure 2: Schematic model of morphological evolution with an increase in the saturation ratio (reproduced with permission of Oaki *et al.*, Crystal Growth and Design 3 (2003); Copyright American Chemical Society).

## b. Controlling Precipitation at a Laboratory Scale

Precipitation is a very interesting synthesis method, because of its versatility. The different steps of the process can easily be modified by the chemist, by simply changing the operating conditions. Nucleation is determined by the saturation ratio  $S_R$ , which controls the number of new solid interfaces. There are different ways to induce supersaturation in a solution. The most common are solvent evaporation, or chemical reactions that produce insoluble species. Starting from a different number of nuclei, particles will grow to attain different final sizes and morphologies; thus by adding a reactive chemical at once or in a continuous way, the final materials may appear completely different. By adding a small amount of fine material to be precipitated (seeds), the apparently chaotic nucleation step can be better controlled. For example, adding calcite seeds allows the precipitation of pure calcite, whereas a mixture of calcite and vaterite with a larger particle size distribution and various morphologies are obtained without seeds (Donnet *et al.*, 2005) (Figure 3 below).

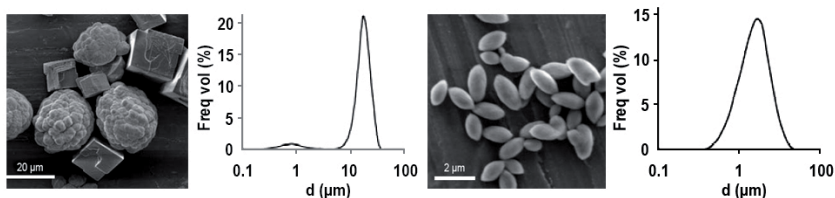


Figure 3: (Left)  $\text{CaCO}_3$ : mixture of calcite and vaterite obtained by precipitation, (Right)  $\text{CaCO}_3$ : pure calcite obtained by precipitation using a seed source (reproduced with the permission of Donnet *et al.*, Langmuir 21 (2005); Copyright American Chemical Society).

Concerning the growth, there are several ways to control this step, by changing the solution composition (pH, conductivity, ionic species, impurities, etc.), or adding organic species. Polymers can be chosen for their specific adsorption capacity on ceramic surfaces. These specific interactions, by inhibiting or promoting crystal growth in some directions, can change the final sizes and morphologies, or even block the precipitation. Many examples can be found in the literature, such as copper oxalate precipitation with a cellulosic dispersant (HPMC) (Jonger *et al.*, 2000; Bowen *et al.*, 2010). These particles become more anisotropic when the concentration of the organic molecule increases, because of preferential adsorption on some surfaces through hydrogen bonding.

Composition of the solution greatly affects the precipitation, such as zinc oxide precipitation at pH 5-6 which follows an agglomeration process leading to quasi-spherical particles, whereas in basic conditions, growth is promoted in one direction leading to anisotropic morphologies (Aimable *et al.*, 2010). Another example is the influence of dissolved species such as complexes. Thus calcium complexes formed with a dispersant (polyacrylic acid, PAA) compete with calcium carbonate precipitation, and inhibit the precipitation at high concentration (Aschauer *et al.*, 2008).

Precipitation is mainly controlled via the *solid/liquid interface*, but the chemist has to work out how to improve the control on materials properties by manipulating and understanding the processing parameters. Microfluidics (Marre and Jensen, 2010) and miniaturized systems allow a very fine-tuning of the nucleation step, better exchange of heat and mass, while lowering heterogeneities in the reactor volume. One example of such systems is a segmented flow reactor with a micromixer for the synthesis of numerous ceramic powders (Aimable *et al.*, 2003): ZnO, CaCO<sub>3</sub>, and BaTiO<sub>3</sub>. This process allows a highly efficient mixing of reactive solutions, in very short mixing times around 10-20 milliseconds. Then segmentation keeps the particles in droplets of small volumes, so that they can grow in a more homogeneous way.

Chemists thus contrive new instruments and set up new devices in order to optimize the chemical agency and the structure of the compound they produce by means of interfaces. They develop new skills and models by trials and errors. Those improvements enable them to understand better what is at stake within interfaces. As Rouse asserts: 'Practices are not just pattern of action, but the meaningful configurations of the world within which actions can take place intelligibly, and thus practices incorporate the objects that they are enacted with and on and the settings in which they are enacted' (Rouse, 1996, p. 135).

The new instrumentation and the up-to-the-minute devices make chemical transformation gain more intelligibility at a finer-grained scale. Chemists can thus reshape the operative and conceptual frameworks within which they model, use, and analyze their chemical bodies. In this respect, interfaces make heterogeneity appear where chemists formerly considered the matter to be homogeneous. They also make dynamic migrations (such as chemical segregations for example) and local reactions come to the fore at the location where chemists previously considered a structure to remain static. Those basic changes renew the way chemical practices are concerned with agency and temporality by means of interfacial interactions between chemical bodies themselves and between scientific communities as well (Llored, 2012). Let us now illustrate how

chemists can find inspiration from natural process to think about interfaces and to connect different specialties around a common research program.

### c. Precipitation at the Interface between Mineral and Living Worlds

Chemists often find their inspiration in the observation of nature. There are many examples of materials precipitated from a biological system; this phenomenon is called “biomineralization” (Meldrum and Colfen, 2008; Mann, 2001). Some very complex structures are obtained at low temperatures and pressures. They display exceptional properties due to a very high degree of organization, following self-assembly processes at the nanometer scale. Chemists find in biomineralization processes innovative strategies to apply to ceramic systems. For example, nacre is a layered, plate-like, composite structure of aragonite (a crystalline form of calcium carbonate) surrounded by an organic matrix of proteins. Its mechanical properties are 3000 times higher than those of pure aragonite, with a relatively simple hierarchical structure, and are better than most synthetic ceramics (Luz and Mano, 2009). Algae and mollusks are able to precipitate their shell at low temperatures and pressures, in a few hours, leading to fascinating structures, such as calcium carbonate shells built by coccoliths, or silica shells built by diatoms (Figure 4). Such structures are attractive for the development of new applications in biotechnology (Sanchez *et al.*, 2005). Finally, bone structure is also an hybrid structure made of an inorganic phase: hydroxyapatite ( $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ ), and an organic phase: collagen fibers. Synthetic materials that copy such structure have been recently developed, which present performances close to natural bones, with a better biocompatibility and mechanical properties (Burdick, 2010).

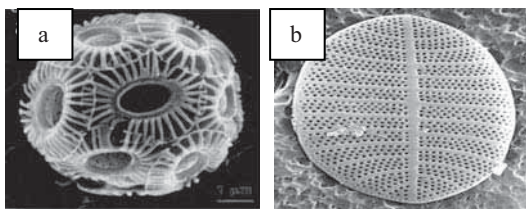


Figure 4: Scanning electron microscopy of (a) a coccolith (scale bar 1 $\mu\text{m}$ , reproduced with the permission of Young *et al.*, Journal of Structural Biology 126 (1999), Copyright Elsevier), (b) a diatom (reproduced with the permission of Lopez *et al.*, Current Opinion in Biotechnology 16 (2005); Copyright Elsevier).

Let us just briefly illustrate one example of biomineralization. Up to now, most of the synthetic preparation methods reported rely heavily on organic solvents and the reducing agents used such as hydrazine and sodium borohydride pose potential environmental and biological risks. At present, to avoid environmental disasters, there is a growing need for chemists to develop nontoxic procedures for synthesis and assembly of nanoparticles such as biomimetic approaches for the growth of advanced materials. Biomineralization processes often imply the formation of nanoparticles or nanocrystals, organized at larger scales via the self-assembly properties of templating macromolecules. It should be also possible to use the synthetic capabilities of living cells for the design of new nanomaterials under mild pH, pressure, and temperature conditions. The common *Anabaena*, *Calothrix* and *Leptolyngbya* cyanobacteria and *Euglena gracilis* are able to form Au, Ag, Pt and Pd metallic nanoparticles and also iron-based nanomaterials such as  $\text{Fe}_3\text{O}_4$  and  $\text{FeOOH}$  of well controlled size and shape (Brayner *et al.*, 2007, 2009, 2012; Dahoumane *et al.*, 2010, 2012; Sicard *et al.*, 2010). Figure 5 below illustrates this intracellular process:

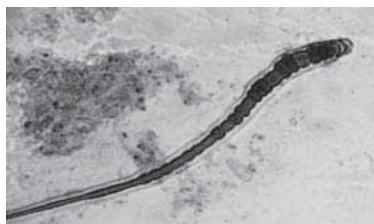


Figure 5: *Calothrix pulvinata* cyanobacteria after production of gold nanoparticles: The cells color changes from green to purple due to the presence of metallic gold nanoparticles inside the cells. Roberta Brayner's courtesy.

The metallic nanoparticles are synthesized intracellularly, and naturally released in the culture medium where they are stabilized by the exopolysaccharides, allowing their easy recovery. *Euglena gracilis* can synthesize  $\text{Fe}_3\text{O}_4$  and  $\text{FeOOH}$ . The magnetic behavior of these “living” materials depends on the nanoparticle structure, size, and shape. Moreover, the size of the recovered particles as well as the synthesis yield is shown to depend on the micro-algae family and genus, demonstrating the flexibility of this approach (Dahoumane *et al.*, 2010). It becomes thus possible to design magnetic akaganeite-cyanobacteria hybrid biofilms. *Anabaena flos-aquae* can produce intracellularly akaganeite ( $\beta\text{-FeOOH}$ ) nanorods by a mechanism involving iron–siderophore complex formation

(Brayner *et al.*, 2009). The  $\beta$ -FeOOH phase is widely used as a precursor in the preparation of ferromagnetic materials such as maghemite ( $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>). To sum-up, the use of solid/liquid interfaces as well as that of biological membranes within the cell are the cornerstones of all those skillful works. On top of that, the multifarious interactions between scientists of different fields are essential at every stage of the process.

#### **d. Precipitation: Concluding Remarks**

Precipitation is a very classical synthesis route, which has a renewed interest from the materials community in recent years because of its simplicity and its versatility. Interfaces are at the heart of this process, during nucleation (creation of a new surface from a liquid phase or from seeds), or growth (depending on supersaturation, or additives which adsorb on preferential surfaces). Innovations have arisen by opening the laboratory to other scientific domains, for example by using microfluidics, or by copying nature and biomineralization processes. Such structures, which are apparently complex, present very high performances against high mechanical, chemical, or thermal constraints. They inspire chemists and ceramists who are trying to copy them to develop nanotechnologies at the interface of chemistry and biology. Moreover, new instruments such as new kinds of microscopy allow chemists and scientists from various fields to deepen their investigation about interfaces and processes.

### **3. Chemistry and Interfaces: From Chemical Practices to Philosophy**

In line with Roald Hoffman (2007), we have done a ‘rotation to laboratory’ in order to grasp what some chemists do and how they construe their knowledge by means of interfaces. Materials chemistry is at the crossroads of multifarious specialties; a careful epistemological study should scrutinize how they interact with one another. *Interface* is thus a useful concept to face the plurality of current chemical practices and it puts the concepts of scientific community and paradigm (Kuhn, 1970) into question. We would like to draw two main conclusions from our present study about the role of interfaces within current chemistry. The first deals with the way science and scientific changes are made intelligible by philosophers and epistemologists. What about the way chemistry evolves? What about the way communities of research change?

We have presented the examples of materials chemistry and sustainable chemistry, but we could have chosen quantum chemistry and other fields

as well. As a matter of fact, Ana Simões and Kostas Gavroglu make obvious that quantum chemistry is neither physics nor chemistry but a true novel specialty which intertwines chemistry, physics, pure and applied mathematics, and computer engineering (Simões & Gavroglu, 2011). Their book, *Neither Physics nor Chemistry*, illustrates and widens many of their previous works in which they established that the emergence of quantum chemistry is the convergent result of divergent scientific traditions (Simões & Gavroglu, 1997; Simões, 1993). In line with them, Llored and Bitbol point out, in this volume, how the entanglement of scientific knowledge and know-how allows to set-up innovative methods in order to study chemical reactivity. Quantum chemistry is envisaged as an open-ended network that encompasses composite approaches and styles held together for studying chemical transformation. Quantum calculations can be considered to be “interfacial” in so far as the Variation Principle mostly used in molecular orbital or DFT calculations needs data from the molecule (structure), its parts (electrons, nuclei, atoms, and so on), and its surroundings (solvent or electromagnetic fields) to reach convergent outcomes. The weighting coefficient that precedes an atomic orbital within a molecular orbital is calculated by means of the procedure of energy minimization that depends itself, directly or not, on the molecular surroundings (Llored, 2010). In this respect, quantum chemistry as a specialty and quantum chemical methods of calculation depend on a host of interfaces. In the same vein, Caillol as well as Rico-Lattes and Maxim clearly point out that sustainable chemistry emergence and development can be analyzed by means of interfaces between specialties and networks (please refer to their respective papers within this volume).

The concept of frontier between two ready-made “disciplines” is useful but of lesser interest than that of interface in order to study how chemists and other scientists interact with one another within a particular project and how innovation and change occur. Frontiers are about “territories” and flux between them. Interfaces are about the dynamic interrelations between the form and the characterizations of this “in-between space” and its surroundings. It is about the “inside” and the “outside” of the specialty at the same time. Interfaces deal with the *co-emergence* of chemical bodies or communities (that is to say with their interrelations) without reifying them as independent from their context. The interface is in-between. In being so, it is thus doubly conditioned by what it first consists of and by the surroundings (social or physical) with which it interacts. Interface both separates and intertwines the two universes that enter into contact within it. It enables a fruitful convergence of the two (Dagognet, 2007). To sum-up, interfaces emphasize the dynamic aspect of the transformation.



If one wants to understand how chemistry is evolving, she needs to identify the economic, societal, and environmental drivers for change. In this respect, one should understand chemistry as deeply embedded in a society and interrelated to it. Moreover, this society defines the meaning of the word “environment” and the laws and norms that limit chemists’ action upon it. Following this line of reasoning, we cannot describe chemistry as an autonomous science oriented only by “paradigms” (Kuhn, 1970) nor do we consider it to be merely propositional. On the contrary, we choose to investigate it as an *engaged* science (Rouse, 1996) that comes to grips not only with social and political requirements but also with the needed co-evolution between industry and academic research. In this respect, interfaces are essential and should be scrutinized from different perspectives (scientific, sociological, historical, or philosophical, to quote but a few).

Sustainable chemistry is not a delineated field but encompasses heterogeneous ways of doing chemistry from nanochemistry to chemical engineering. All those chemists mostly use the same molecular representations, but they do not have the same chemical culture and know-how. Moreover, they do not use the same resources in the same sites with the same aims: their scientific “forms of life” differ, to refer to the second Wittgenstein (1997). The unity of sustainable chemistry is the result not of a strict identity or of a unique reference but, on the contrary, that of a network of overlapping resemblances none of which run through the totality. It is the *conjunction* of those forms of life that is subsumed under the label “sustainable chemistry” (Llored, 2011). It is precisely what Maxim and Rico-Lattes demonstrate when studying how French chemical communities, which previously existed within separate fields, became involved in the French interdisciplinary program “Chemistry for Sustainable Development” developed since 2006 (Maxim and Rico-Lattes, 2012). The dynamic overlaps of diverse chemical networks generate new similarities and make it possible for a large collection of chemical processes, green metrics, environmental norms, and new instruments to co-exist and to co-evolve within various research projects. Those open-ended interfaces challenge the concepts of “field autonomy” and “unique paradigm” assumed by some philosophers (Llored, 2013a).

We need to study how scientific concepts circulate between different fields. Some concepts come from other fields, such as sustainable development, ecology, and ecodesign. They are then translated into the green chemical schemes. Others come from sustainable chemical practices such as atom economy, life cycle analysis, and ecochemistry. Assigning new meanings, new roles within hierarchies, and new relevant goals,



methods and taxonomies to the different protagonists and institutions involved in the process, is an “immanent process of deterritorializations and reterritorializations”, to use Deleuze and Guattari’s terminology (1987). According to them, a concept does not require only one problem under which it alters or replaces preceding concepts, but, rather, a crossroads of problems within which it is combined with other coexistent concepts (Deleuze and Guattari, 1991).

Isabelle Stengers asserts that a scrutiny of a scientific “event” is basic for grasping scientific novelty and evolution without reifying them by means of simple reductions and deductions, and without accepting ready-made philosophical dichotomies. We have to follow the process in so far as the process is precisely what is at stake (Stengers, 2000). This openness of practices should be integrated into philosophical and epistemological studies of scientific processes. Joseph Rouse asserts:

As a result, practices are radically open: whether a subsequent action counts as a continuation, transformation, deviation, or opposition to a practice is never fixed by its past instances. These instances are, of course, relevant to the identification and continuation of a practice, but they cannot be decisive in settling whether new cases exemplify the practice; the new cases themselves may, after all, constitute a reinterpretation of their predecessors. Social constructivists’ interpretations of practices fail to take adequate account of the openness of the social dimensions of practices. When they insist that social relations or interests are explanatory, they foreclose the possibility that those relations or interests, or even their characterization as social, may be what is at issue in the continuation of the practice (Rouse, 1996, p.141).

We uphold that the study of chemistry needs to take interfaces into account in order to grasp the radical openness of practices. Chemistry is a language as well as a field of practices revolving around instruments of all kinds. We call for a pluralistic approach of science within which interfaces are studied by a “rotation to laboratories”. As Andrew Pickering claims:

[T]he idea that each scientific community has one big paradigm serves to conjure up a boundary around science—it makes it possible to think about science as a self-sufficient and self-contained entity. [...]. [J]ust where the boundary lies between the inside and the outside of any given science becomes a matter for historical enquiry rather than a priori philosophical resolution (Pickering, 2001, p.506).

He adds:

[T]he center of gravity lies elsewhere, at the point of intersection of human and material agency. The trajectory of evolution of the social has here to be understood in terms of emergent resistances and accomodations at the *interface*<sup>1</sup> of these heterogenuous realms (Pickering, 1995, p.168).

In her contribution to this present volume, Bernadette Bensaude-Vincent develops an idea previously developed in the book that she co-authored with Jonathan Simon (2008) *Chemistry the impure science*. They made a strong argument for the philosophical interest of chemistry based precisely on the fact that it is an “impure science”. “Impure” not in a sense related to the pollution originated from chemical activities, but because chemistry challenges the *purified image* of science as a discipline mainly guided by a strong paradigm and for the most part autonomous from the other sciences, technology, and the society. According to Bensaude-Vincent, the epistemological specificity of chemistry and its related ontology are closely dependent on its “impurity”. In this respect, science is not separated from technology, but is not just a mere mixture in various proportions of the two. She refers to the Aristotle’s “mix” to illustrate her proposal. A mix is something different from the sum of its components; technoscience is thus something different from both science and technology. Conversely, an “aggregate” is a mere additive combinations of elements and their properties that retains the properties of the components.

Following this description, we can draw a parallel with multidisciplinary projects that assemble agents (be they human or not). Various fields of practice and research are sometimes “mixtures” and not merely aggregates. Emergent pratics, processes, and concepts can be contrived from within ongoing interactions. They can, nevertheless, cease to exist and sometimes return to their prior states as soon as the common project ends, because of lack of funding, ecological disaster, reorientation of the economic, and political or scientific choices. New processes, methods, and compounds become manifest according to their effectiveness for possible sustainable action. In this respect, chemists’ activities depend upon their chemical consequence and the feedback coming from the world and the rest of society. Emergence, temporality, interfaces and agency appear then as co-dependent tools with a strong heuristic power for thinking about sustainable chemistry as a field of practices that encompass large domains of activities, be they scientific or not. We suggest the mixture/aggregate dichotomy should be an interesting tool for thinking about the ways in which chemical agency is evolving.

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<sup>1</sup> Our emphasis.

Stengers and Bensaude-Vincent conclude their *History of Chemistry* by following Diderot's approach of "chemical terrains". Their ongoing experience within a particular terrain enables chemists to identify relevant questions and to understand what is at stake in their activities. Chemists' labour is an "art of circumstances" that has nothing to do with the systematic deduction from the standpoint of a law of nature (Bensaude-Vincent and Stengers, 1996). The authors assert that the identity of chemistry lies in the "solidarity" between the terrain and the chemists. They do not understand science as a set of autonomous territories but rather as the result of open-ended interactions embedded in the society. In his contribution to the present volume entitled *The Tao of Chemistry* Pickering goes on say that:

Chemical knowledge, one can say, grows as part of a heterogeneous material, social and conceptual assemblage—increasingly an integral part of that assemblage, but never its controlling or generative centre as traditional history and philosophy of chemical ideas implicitly suggests. And the philosophical and historiographic moral of this is that we can never get a secure grip on what chemical knowledge is without at the same time taking account of the specific flows and transits and the wider socio-economic assemblage with which it engages.

This is not how we end this article because we would like to draw a second main conclusion from our present introductory work about current chemistry and interfaces. In line with Dagognet, Gérard Chazal highlights that, up to a certain point, a "dialectics of mediation" lies behind the concept of interfaces and makes us draw our attention to the particular *substrates* which allow our messages, information, knowledge, and the things themselves, to circulate. The chemical body itself as a substrate cannot be eliminated (Chazal, 2002). Form is as important as the content; they are co-dependent and co-defined from within interfaces. The new microscopic techniques point out this co-dependence when studying a catalytic process sensitive to the occupation of specific sites at the interface between two *media*.

This kind of new materialism is in keeping with what new instrumentations "afford". In his contribution entitled *Hinges and Affordances. New tools in the Philosophy of Chemistry* belonging to the last part of this volume, Rom Harré defines affordances as displays produced by specific human manipulations of an actual locally constructed apparatus. To sum-up, 'the way an activity is examined creates its distinctive picture, realizing certain affordances while excluding the manifestations of others' (Harré, 2006). Affordances are certainly products of the interaction of equipment and the world, but in many cases they are

not constituents of that which affords them, neither as properties such as “colour” nor as entities such as “parts”, nor as processes such as “walking” or self-molecular assembly. Chazal, Dagognet, and Harré defend the idea of the non-exhaustiveness of matter. The characterization of matter is instrument-relative. It does not ‘reveal’ any intrinsic, say, any monadic properties (Harré and Llored, 2013). Affordance is an *interfacial* concept that focuses on the result of an interaction, say, on a phenomenon. Dagognet calls for a “rematerialization” considering that matter as an active material and not as an inert and geometrized set of basic particles (Dagognet, 1989). Chemists consider matter from within an ontological and pluralistic point of view. Chemical individuals (molecules, materials) are active bodies defined by means of chemical operations and are classified according to their reaction with other bodies. Chemical individuals are thus defined by means of networks of interdependencies. The characterization of a chemical body does not refer to an “essence” but to its relations with other chemical bodies or with photons. Chemical reactivity is thus context-sensitive. It depends on the device, the parameters being used, the way reagents are added, but also on specific instrumentation, and on interfaces! The interfaces constitutively influence the process and the transformation. In this respect, they enter into the very characterization of the chemical body being synthesized or analyzed in so far as chemical bodies require chemical operations in order to be identified. A chemical body is the result of a purification requiring acting upon matter to disentangle it. Chemist need relations to define chemical *relata* but they also need to purify mixtures to obtain new *relata* that enable them to afford new relations. Chemistry faces the philosophical debate about the relation/*relata* priority. Chemists co-define *relata* and relations in order to transform the world as Llored and Bitbol point it out in their paper in the second part of the present volume. The interfaces are now at the forefront of this chemical strategy because of new instruments and technology. Chemical transformations can be studied at finer and finer-grained scales. Interfaces are multiplied at different scales. Heterogeneity is flourishing in pair with our increasing power of action over the world (Llored & Harré, 2013). According to us, chemistry is relevant for analyzing science as a special kind of socio-historical practical activity. In this respect, interfaces are of importance to deal with scientific innovation and change while providing stark arguments in favor of a chemical ontology.

Let us nevertheless consider this collective work as a simple *tool* tailored to encourage deeper and wider forthcoming works and to stimulate stronger cooperation between philosophers and chemists. The concept of interface deserves to be looked at in somewhat more detail, and

especially the way chemists define and use latent heats, nucleation theory, or the differences between solids and liquids. All those definitions are much more problematic than this preliminary paper suggests. We also think that before one further develops analogies between physical interfaces and interfaces between disciplines, one needs to address more deeply what an interface is and the limitations of the concept. There is the concept on the one hand, and its metaphoric use on the other. That is why the study of chemical practices remains of crucial importance. A deeper investigation that tackles all those questions is in process (Llored, 2013b).

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# CONCLUSION: CHEMISTRY AS PRACTICE

## ROM HARRÉ

In line with the innovations of Wittgenstein's later philosophy (Wittgenstein, 1953) it is illuminating to look on the role of chemists as the working through of a repertoire of practices. A practice is an established and repeatable pattern of actions with an intended outcome and which is shaped or disciplined by changing norms of correct procedures. Some norms will change slowly, and some rapidly. The laboratory is the home of the constituent material practices of chemical experimentation. Philosophers have much to say about the nature of what is in the laboratory, the *instrumentatrium*. Explanations in chemistry and particularly their integration with classification systems in the periodic table illustrate another kind of practice.

Bruno Latour (1987) has given us the nice metaphor of laboratory equipment as assistants in the work of promulgating the opinions of chemists and popularizing their views on what they have produced by their manipulations of that equipment.

Accepting the principle that chemists are motivated to use equipment to support their claims in the society of chemists, there remains a fundamental distinction in the way the equipment is related to the world. Some pieces of equipment, let us call them instruments, are used to detect states of the world and to differentiate the substances to which they are applied, such as indicators, gas chromatographs, and so on. Other instruments are used to measure metrically defined states of the substances of the world. Both kinds of instruments are *causally* related to the world. There can be ancillary research projects to examine such causal relations in the refinement of instruments both as detectors and as measuring devices. The other kind of equipment we could call 'apparatus'. With apparatus we abstract and isolate chemical processes from complex environments that can make their study confused or even impossible. An apparatus is related to the world by a conceptual relation—analogy. The apparatus is analogous to some environment but set up in a much-simplified form. While we can discuss the accuracy of instruments it

makes no sense to reflect on the accuracy of apparatus. Instead questions addressed to its value in knowledge gathering concern how verisimilitudinous it can be, that is how convincing is it as a model of something that happens in the world, something which is usually embedded in a complex array of other processes.

The power of chemistry as a repertoire of knowledge producing practices concerning material stuffs has meant that it has played a role in many other sciences—geology, biology, geography and so on. Such applications have not been queried by sceptical philosophers. However there is one science in which the role of chemical knowledge and techniques has been questioned and there are many who regard it as conceptually incoherent. This is the attempt to redefine and to explain psychological phenomena in chemical terms. Two main arguments have been given for this strong conclusion. The mereological argument asserts that using a concept the meaning of which is determined by its use of a whole being for a part of that being is a fallacy. So use the word 'remembers' to describe the hippocampus is a fallacy since the word gets its meaning from its use to describe a whole person. Another argument is built on the principle that psychological concepts applied to persons have a moral or normative aspect which is lost if those concepts are applied to human bodies and their parts. Thus a person can be 'depressed' but 'depression' is not replaceable with 'low serotonin concentration'. That low serotonin concentration in the synapses has anything to do with depression requires us to already be able to recognise depression. So a chemical account of depression cannot be an alternative 'scientific' description of depression.

As an 'exact science' does chemistry give us a faithful representation of the world of material substances and the methods by which they may be transformed? This may seem a very naive question until we reflect on the way that what we can find out about the world depends on the apparatus we have available and the techniques we have for using it. Philosophers have begun to draw on the psychology of perception for a concept with which to express the inextricability of experimental practices and the available *instrumentarium* in the results of empirical studies. J. J. Gibson (1967) invented the word 'affordance' to describe what something displays when acted upon in a certain manner. A material thing, say a tennis ball, will display many different properties depending on how a person interacts with it. Prompted by a deservedly famous paper by J. Earley (2005) questioning whether the salt that sea affords is properly to said to be constituent of it, a deeper issue has been raised—are the products which are the affordances of certain kinds of interventions in the material

world, such as electrons, properly to be described as constituents of atoms? Can we always justly read back along a kind of mereological chain from affordances to constituents? This question prompts further reflection on the status of atomic and subatomic hypotheses in chemical theory. This may be another context in which treating atoms as constituents of models of molecules and electrons and other particles as constituents of models of atoms, rather than their real parts.

This short conclusion is meant to point beyond the topics of this book towards a continually expanding range of philosophical topics that the revival of interest in this fascinating field opens up.

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Methodologies :  
How to Study  
Chemistry ?  
*Part II*



# **HISTORICAL APPROACHES**

# PHILOSOPHY OF CHEMISTRY: WHERE HAS IT BEEN AND WHERE IS IT GOING

ERIC SCERRI

## **Introduction: The Philosophy of Chemistry as an Academic Discipline**

Jean Pierre Llored the organizer of the Paris meeting has asked me to say some words of introduction concerning the relatively new field of the philosophy of chemistry. This I will try to do as well as discussing the way that the field has progressed in various countries over recent years.

Many authors have sought to locate the origins of the philosophy of chemistry. This is not an easy task. Of course there have always been authors who were drawn to the more thoughtful, more fundamental aspects of chemistry who can be said to have been doing philosophy of chemistry throughout the ages. Moreover, it is well known that with the development of modern atomism starting with John Dalton, the field of chemistry became rather philosophical as it seemed to be dealing with the ultimate constituents of matter.

Nevertheless it is to the modern period that we must turn if we are to find the development of the sub-discipline of the philosophy of chemistry with its own international society, regular conferences, books and journals. Let me briefly touch on these aspects.

I believe it is fair to say that in the English speaking nations the philosophy of chemistry as a communal activity began to take shape as a result of the Yorkshire-born chemist Michael Akeroyd. Akeroyd who had already published a few articles dealing with philosophical aspects of chemistry, noticed that several authors around the world were spontaneously starting to publish on philosophical aspects of chemistry. Akeroyd therefore decided to organize an international symposium on the subject and this took place twice in his own city of Ilkley in Yorkshire in the early 1990s.

At this time I was finishing a PhD thesis under the supervision of Heinz Post at King's College London. At a festschrift celebration held for Post at a London restaurant I found myself sitting next to the late Annie

Kuipers from Kluwer, who were the publishers and sponsors for the festschrift. When Annie turned to me at the dinner and asked what kind of work I was doing, I replied that I was working on the philosophy of chemistry. At this point she asked me whether there existed any journal for this field and when I responded that there was not, she immediately decided that we should start one. After several years of formal proposals and planning the *Foundations of Chemistry* started to publish three issues per year in 1999 by which time I had moved to the US.

Meanwhile, the two meetings that Akeroyd had organized as well as the evolving journal prompted us to formalize our international society for the philosophy of chemistry or ISPC, which began to hold annual meetings in 1997.<sup>1</sup>

In fact I later discovered that there had been another journal for the field, called *Hyle*, which began as a newsletter for German chemistry educators interested in foundational issues and which then grew into an on-line journal. This journal was eventually also issued in hard copy form, although never distributed by a mainstream publishing house.<sup>2</sup>

When it comes to books I would like to mention the monographs by Jaap van Brakel, Joachim Schummer, myself (Scerri, 2008, Schummer, 1996, Van Brakel, 2000). There are also some edited collections, some of which arose from conferences, including Earley; Baird, Scerri and McIntyre and Bhushan and Rosenfeld, although this is not intended to be an exhaustive list (Baird, Scerri, McIntyre, 2006; Bhushan, Rosenfeld, 2000; Earley, 2003).

The philosophy of chemistry is generally well represented at mainstream philosophy of science conferences such as those of the Philosophy of Science Association whose meetings are held every two years in North America. In addition articles on the philosophy of chemistry have appeared in numerous encyclopedias and dictionaries for philosophy and philosophy of science. So much for a brief round up on the Anglo-American scene.

As to progress in the French speaking world, I am not really in a good position to comment except perhaps to mention the work of the historian-

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<sup>1</sup> The following official meetings of ISPC have been held; Ilkley, UK (1997), Cambridge, UK (1998), Colombia SC, USA (1999), Poznan, Poland (2000), Loughborough, UK (2001), Washington DC, USA (2002), Tartu, Estonia (2003), Durham, UK (2004), Knoxville, TN, USA (2005), Split, Croatia (2006), San Francisco CA, USA (2007), Coburg, Germany (2008), Philadelphia PA, USA (2009), Oxford, UK (2010), Bogota, Colombia (2011), Leuven (2012).

<sup>2</sup> The editor remains as Joachim Schummer, who is currently living and working as an author in Berlin.



philosopher Bernadette Bensaude-Vincent who was been working in the field even before the revival that took place in the early 1990s in the UK and US. Bensaude-Vincent has been well aware of the developments in the Anglo-American approach and has become increasingly critical of them. Since part of the purpose of Jean-Pierre's meeting is to bring about a rapprochement among us I would like to address this issue briefly because I sincerely believe that we can all benefit from adopting a more mutually tolerant attitude concerning our various approaches.

But before doing so, and as other authors have already noted, it must be conceded that the philosophy of science as practiced in France has for a long time drawn rather heavily from chemistry in a manner that is almost completely absent in Anglo-American philosophy of science. I am referring to the work of such noted authors as Duhem, Meyerson, Metzger and Bachelard.

### **Bensaude-Vincent's critique of Anglo-American philosophy of chemistry**

Bensaude has recently written,<sup>3</sup>

Le dédain des philosophes pour la chimie n'est donc pas étranger à un projet de subordination voire la réduction de la chimie à la physique. Mais il a été favorisé également par le positivisme logique porteur d'un projet d'unification des sciences par adoption de la 'langue de la physique' comme langue universelle. Or ce projet, fortement critiqué par plus d'une génération de philosophes, a été abandonné. La 'désunité' des sciences et même devenue une revendication philosophique majeure à la fin du XX<sup>e</sup> siècle. Il est temps enfin de reconsidérer ce qui peut fonder l'originalité d'une science comme la chimie (Bensaude-Vincent, 2008, p.16).

The reason why physics has been adopted as a form of universal language has little to do with philosophers of science such as the logical positivist school. The reason lies rather in the tremendous success that

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<sup>3</sup> The disdain of philosophers towards chemistry is not therefore out of place within the context of a project in which chemistry is seen as being subordinated by physics. But this disdain is equally favored by logical positivism that brings a project of unification of all the sciences through the adoption of a common language of physics as the universal language. However this project has been strongly criticized by a generation of philosophers and has been abandoned. The "disunity" of science has even become a major philosophical movement at the end of the twentieth century. It is finally time to reconsider what could be the foundation of the uniqueness of a science like chemistry. (Translation by Eric Scerri)

physics has had in providing a fundamental description of many phenomena in other fields, especially in the field of its closest scientific neighbor, namely chemistry. Although one can argue about the finer points of the extent to which the reduction of chemistry has succeeded the overall success of this enterprise is completely and utterly undeniable.

I will give just one example. When the periodic system was discovered in the second half of the 19<sup>th</sup> century there was no underlying explanation for this pattern or representation that connects all the elements together into a coherent whole. The twentieth century saw the discovery of the electron, the structure of the atom including the structured manner in which electrons circle the nucleus of atoms. With this information a succession of ever more sophisticated models of the atom starting from Bohr, and culminating with Schrödinger and Dirac, have provided a causal explanation of why the periodic table is the way that it is and for why the elements belonging to a particular group in the table behave in a similar manner.

Bensaude-Vincent is correct in claiming that the philosophical school of logical positivism has become outmoded. The particular way in which these philosophers believed that various branches of science reduced to physics may well have been found to be wanting. Nevertheless, the understanding of chemical phenomena that has been provided by physics is everywhere to be seen in modern chemistry. Even if epistemological reduction has not been achieved in a smooth fashion as the logical positivists might have wanted, the ontological reduction of chemistry is observed on a daily basis in the more physical and theoretical branches of chemistry.

Here is another quotation from Bensaude-Vincent and from the same book,

...Car l'une des motivations principales de ce timide regain est de lutter contre les préjugés qui ont fait de la chimie une sorte de physique appliquée. Certains chimistes semblent toujours souffrir du trop fameux jugement émis en 1929 par l'un des fondateurs de la mécanique quantique, Paul Dirac: 'les lois physiques sous-jacentes nécessaires à la théorie mathématique d'une grande partie de la physique et de la totalité de la chimie sont ainsi complètement connues, et la seule difficulté restante est que l'application exacte de ces lois conduit à des équations trop compliquées pour qu'on puisse les résoudre' (Bensaude-Vincent, 2008, p.18).<sup>4</sup>

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<sup>4</sup> ...Though one of the main reasons for this tentative return is to fight against the prejudices that have made chemistry a kind of applied physics. Certain chemists seem to still suffer from the too famous judgment proposed in 1929 by one of the

Bensaude-Vincent seems to believe that the founders of the philosophy of chemistry as somehow trying to reclaim chemistry from the jaws of the reduction that is being carried out by physicists. In fact this is not the case, although I can only really speak for my own work. As a philosopher of science I adopt a more agnostic, and less partisan, approach than Bensaude-Vincent seems to attribute to the new wave of philosophers of chemistry. I have no vested interest in showing that chemistry is not in fact reduced to physics. I am rather interested, to repeat, in the extent to which it is so reduced. This is because part of my work is motivated by the manner in which chemistry is presented in today's chemistry textbooks. In this context the impression gathered is that the reduction is complete, something which I believe to be the wrong message to convey to students and more importantly not a reflection of the true state of affairs. But the degree to which particular phenomena or branches of chemistry are illuminated by physics is a matter best addressed by the chemists working in such areas and not by outsiders, like Bensaude-Vincent, who study rather watered-down accounts of the scientific issues and what one or other particular school of philosophy may have to say on the question of reduction. It should also be said that it is only some schools of modern philosophy of science that has abandoned all hope of reduction in the way that Bensaude-Vincent implies is the norm among philosophers of science working today. Returning to Bensaude-Vincent's review of the development of Anglo-American philosophy of chemistry she has also written,

Ainsi le journal crée par Eric Scerri en 1999 est-il largement focalisé sur les problèmes de réduction de la chimie à la physique. Le titre même du journal semble une réponse de la communauté chimique à la longue tradition d'ignorance de la chimie dans *Foundations of the Unity of Science*, célèbre publication des positivistes logiques (Bensaude-Vincent, 2008, p.18).<sup>5</sup>

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founders of quantum mechanics, Paul Dirac: "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws lead to equations much too complicated to be soluble". (Translation by Eric Scerri)

<sup>5</sup> In this way, the journal founded by Eric Scerri in 1999 is largely focused on the problems of reduction of chemistry to physics. The title of the journal itself seems to be a response from the chemical community to the long-standing neglect of chemistry in *Foundations of the Unity of Science*, the celebrated publication by the logical positivists. (Translation by Eric Scerri)

This is one subject on which I think everyone must agree I can speak with complete authority since I was responsible for the choice of the title of the journal. I did not choose the title because I regarded modern philosophy of chemistry had been dominated by logical positivism and that the neglect of chemistry was necessarily due to the influence of this school. As I indicated above, the neglect of chemistry is partly justified on the grounds that broadly speaking chemistry has in fact been reduced to physics and for philosophers interested in fundamental aspects of the subject it makes some good sense to concentrate on physics.

My reason for choosing the title that I did was rather because I wanted to found a journal that was analogous to the long-standing journal called *Foundations of Physics* in which physicists as well as philosophers of physics could write about what they regarded as foundational issues. There was no philosophical commitment, nor was there any attempt to combat the philosophy of any previous school of philosophy. There was absolutely no connection with *Foundations of Science* à la Logical Positivism.

On the question of whether the journal has indeed been “largement focalisé sur les problèmes de réduction de la chimie à la physique”, I can confidently reply in the negative. Of the 149 articles that have been published since the journal began in 1999, at the time of writing, only 16 are concerned with the reduction of chemistry to quantum mechanics, even broadly construed. This represents only about 11% of all papers published in the journal and clearly not evidence of “largement focalisé”.

Bensaude then claims that,

Si la question du réductionnisme est la condition de visibilité philosophique de la chimie, si elle devient le passage obligé pour capter l'attention des philosophes, la philosophie chimique à peine émergée sera elle-même très vite réduite à des problèmes théoriques. La philosophie chimique restera toujours subordonnée à celle de la physique ... (Bensaude-Vincent, 2008).<sup>6</sup>

Indeed, the visibility of philosophy of chemistry does not rest on studies on reduction. Nevertheless I maintain that this is an important question that has many ramifications in chemical education for example. A great deal of my own work has been an examination of the extent of the

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<sup>6</sup> If the question of reductionism is the condition under which chemistry becomes visible, if it becomes the obligatory pathway for capturing the attention of the philosophers, the philosophy of chemistry, which has only just emerged, will be very quickly reduced to a question of theoretical problems. The philosophy of chemistry will always remain subordinate to that of physics... (Translation by Eric Scerri)

reduction of chemistry to quantum mechanics because I believe that chemical educators and chemistry textbooks don't question this aspect to a sufficient degree (Scerri, 1998, 2000a, 2000b). In carrying out such work I have deliberately steered clear of using any criteria for reduction that were recommended by the logical positivists.

My approach has consisted rather of what I term a 'naturalistic approach' in which I examine reduction in the way that a chemist of physicist would pose such a question. Instead of using the logical apparatus that a logical positivist might use I have examined the scientific content more directly. I am not concerned with axiomatizing the theories of chemistry and the theories of physics and in trying to establish bridge principles. This is what logical positivists would have done and it is because I have avoided any such approach that I find Bensaude-Vincent's remarks to be of little consequence to the current state of the new philosophy of chemistry as carried out in the Anglo-American or analytical tradition.

In addition I have worked on the question of the ontological reduction of chemistry, not because I doubt that this is a *fait accompli* but because several philosophers of chemistry, wrongly believe, to my mind that chemistry does not ontologically reduce to physics. "Fait accompli" is not quite the right expression here because ontological reduction does not refer to any human act of reducing one scientific description to that of another level. Ontological reduction refers to the way things 'really are' from a God's Eye point of view as it has sometimes been described. Of course a completely God's Eye point of view is not something that any of us humans can comment upon but there are many philosophers who believe that the way things really are is given to us by our best theories.

Others believe that to study the ontological reduction of chemistry should involve studying whether the entities belonging to the chemical realm can be explained by theoretical physics. This brings me onto the second part of my article in which I will briefly examine the work of a one prominent philosopher of chemistry, Robin Hendry, who in several papers has claimed that chemistry is not in fact reducible to physics, not because of any computational difficulties but, because such a reduction is not possible even in principle.

But before turning to this second part I would like to comment on Bensaude-Vincent's positive recommendation rather than her views on what philosophy of chemistry should *not* consist of. Bensaude-Vincent recommends studying, above all else, the *practice* of chemists in order to discover a philosophy of chemistry. This is of course highly commendable and she has followed this up with a number of major studies on

nanotechnology a new sub-discipline where she sees chemistry increasingly heading. Needless to say, the study of practice can provide an interesting historical and sociological perspective of any field of science but can often miss the all-important content of the science. This has become only too obvious as a result of the more egregious studies to emerge from the 'Science Studies' and the Sociology of Scientific Knowledge (SSK) programs. In such circles some have even ventured to claim that it is better if the researcher does not understand too much of the science in question so that he or she may remain fully impartial and objective, although even any talk of "objectivity" would probably be viewed with great suspicion.

Philosophy of chemistry, I claim, is as much about the contents of the chemical world (the chemical ontology) as it is about how chemists go about doing their work. Of course the two aspects are intimately related but I suggest that the first is as important as the second activity. The second activity, as I have just suggested, can easily lapse into studying all manner of sociological factors, while omitting the actual science involved.

But surely there is room for the study of all these areas, from reduction of chemistry to physics all the way to the sociology of chemistry and chemical practice.

Why limit the field at such an early stage? The emerging field can hardly afford these divisions. There is no denying that journals like *Hyle* and *FOCH* have given the field visibility and that many mainstream chemists and physicists have been drawn into the field. What we need now is to consolidate and move forwards together.

Enough, I say, of this Anglo-American-French rivalry that is perhaps a reflection of the long-standing analytical-continental divide in general philosophy.

This is why the meeting organized by Jean-Pierre Llored has been a very important one, since he too believes in a spirit of reconciliation among philosophers of chemistry and he is somebody who embraces both analytical aspects as well as the study of chemical practice.

## **Ontological Reduction of Chemistry**

As mentioned above, the reduction of chemistry has been an important topic in the emerging philosophy of chemistry, although not quite as important as Bensaude-Vincent would have us believe. Moreover the question of reduction has been mostly confined to asking about the epistemological reduction of chemistry by which I mean the question of whether theories of chemistry have been reduced to theories of physics.

Some authors prefer to call this study theoretical reduction to avoid the possible confusion that the label ‘epistemological’ might bring.

There has also been some work on the question of ontological reduction, although again various authors have a different understanding of what this might mean. (Lombardi and Labarca, 2006; McLaughlin, 1992; Le Poidevin, 2005; Hendry, 2010) Lombardi and Labarca have claimed that ontological reduction is a more important question. This is not unreasonable since it addresses the more general question of whether chemistry is reducible to physics in principle rather than just in practice. If one remains on the question of theoretical reduction it might always be the case that the present theories of chemistry or of physics or both are not sufficiently well developed in order to establish reduction. Alternatively it may be that the theories are perfectly adequate but that nobody has been able to show that reduction goes through. The question of ontological reduction need not suffer from these practical limitations since it claims to address the question in principle. Whether this can realistically be assessed is something that I doubt, but I will nevertheless assume that it may be possible in order to consider the last of the above named authors, Robin Hendry, who bases his conclusions upon the Born-Oppenheimer approximation and the notion of ‘structure’ in chemistry.

Hendry correctly points out that,

... reductionists and non-reductionists can agree that classical inter-theoretic reductions of chemistry are not currently available, but will differ in how they interpret the situation. As long as reduction is seen as a dated inter-theoretic achievement, however, the issue is essentially future directed—both sides must wait and see... (Hendry, 2010, p. 184).

I also agree completely with his saying that,

... we [need to] separate the inter-theoretic and the metaphysical aspects of the reduction debate: the former concern the explanatory relationships between theories and the latter the relationships between their subject matter. This separation is necessary because there are reasons why the inter-theoretic reduction of a special science may fail that are quite independent of any metaphysical relationship between physics and the special sciences (Hendry, 2010, p.184).

The first reason that Hendry suggests can produce a failure of theoretical reduction but not necessarily ontological or metaphysical reduction is that quantum mechanics, the reducing theory is highly abstract, and that any chemical case in question is rather specific and

necessitates the use of approximations of all kinds. It is possible that any failure of reduction can be blamed on this move and if so, reduction would have failed on epistemological or inter-theoretical grounds. One could not conclude that there is a lack of ontological reduction.

The second reason he suggests is that two scientific disciplines, such as chemistry and physics, typically develop independently as history unfolds and that there is no guarantee that the two sciences mesh together in such a way that reduction can be demonstrated. Once again any apparent lack of reduction can be attributed to inter-theoretical issues and cannot rule out the ontological reduction of one level to another one.

In order to articulate a form of ontological reduction we need to look elsewhere and Hendry then turns to this more difficult task. He writes,

One obvious requirement on a criterion of ontological reduction is that whether or not it obtains must be a substantive metaphysical issue that transcends the question of what explanatory relationships exist between theories now, or might exist in the future, even though inter-theoretic relationships must continue to be relevant evidence (Hendry, 2010, p. 184).

In saying this I believe that Hendry is already opening the door to possible complications since it is not clear to what extent inter-theoretical relationships must continue to be relevant and at what point in such considerations one might have lapsed back into a discussion of theoretical reduction. To the present author, it looks suspiciously like Hendry is trying to 'have it both ways'. On one hand the claim is that theoretical issues cannot have too much bearing on ontological relations while, on the other hand, Hendry accepts that we get our ontology from our theories. Be that as it may, let us see how Hendry wishes to proceed.

Hendry then writes,

Reducibility is at the strong end of the spectrum because it is the limiting case that denies the distinct existence of what is dependent—the reductionist slogan is that *x* is reducible to *y* just in case *x* is 'nothing but' its reduction base, *y*. ... a consensus has emerged in recent philosophy of mind that the relevant aspect should be causal. Alexander's dictum is the principle ... according to which *being real requires having causal powers* (Hendry, 2010, p. 184).

In this way, Hendry following Alexander makes, a connection between the question of causation and that of reduction. But notice that as Hendry concedes, this is only one option. Moreover, the fact that a consensus may have arisen in the philosophy of mind may, or may not, be relevant to research in the philosophy of chemistry. And any connection established



in the philosophy of mind is of *even less relevance* to chemists and physicists trying to grapple with the question of whether chemistry is ontologically reduced to physics. But let us also grant Hendry this connection and see where it might lead him.

The ontological reductionist thinks that special-science properties are no more than their physical bases because the causal powers they confer are a subset of those conferred by their physical bases; the emergentist sees them as distinct and non-reducible just because the causal powers they confer are not exhausted by those conferred by their physical bases. The additional causal powers are exerted in downward causation (Hendry, 2010, 185).

Hendry thus characterizes emergentism as invoking downward causation—namely that the special-science properties sometimes push their physical supervenience bases around. He also claims that ontological reductionism assumes the causal closure, or completeness, of the physical, meaning that physical effects are brought about solely by physical causes via physical laws. At this point Hendry appeals to the work of C.D. Broad on emergentism and claims that Broad's work provides,

...an account of emergence from which a model of downward causation is *readily extracted* (Hendry, 2010, p. 185). [my italics]

Broad's account of the disagreement between pure mechanism and emergentism is *easily formulated* within quantum mechanics, in which the motions are governed by Hamiltonian operators determined by the forces acting within a system (Hendry, 2010, p. 185). [My italics]

This seems to be a rather odd statement given that much work in the philosophy of physics has aimed at identifying whether reductionism breaks down in the context of quantum mechanics and the findings have been notoriously inconclusive. But here now Hendry informs us that drawing on the writings of a philosopher in the 1920s, the identification of emergence in an entirely different field of quantum mechanics becomes a *simple* matter.

But again let's see where he goes with this,

Where does downward causation fit into this? For the emergentist, every complex system is composed of the same basic stuff, but some complex systems are covered by non-resultant or configurational Hamiltonians. In an emergent complex system, the behaviour of the basic stuff of which it is made is governed by a *configurational Hamiltonian*, which is different

from what it would be were its behaviour governed by the resultant Hamiltonian (Hendry, 2010, p. 185). [My italics]

By now the reader must be eagerly asking where these configurational Hamiltonians that Hendry claims occur in quantum chemistry might be. It is for this reason that Hendry turns to molecular quantum mechanics and in particular the use of the Born-Oppenheimer approximation. Before going too far forwards it is necessary to consider the contents of this approximation. For example, a well-known author on quantum mechanics in chemistry writes,

The Born-Oppenheimer approximation supposes that nuclei, being so massive, move much more slowly than the electrons, and may be regarded as stationary. This being the case, we can choose the nuclei to have a definite separation (i.e. we can choose a definite bond length) and solve the Schrödinger equation for the electrons alone; then we can choose a different bond length and repeat the calculation. In this way we can calculate how the energy of the molecule varies with bond length (and in more complex molecules with angles too), and identify the equilibrium geometry of the molecule with the lowest point on this curve. This is far easier than trying to solve the Schrödinger equation by treating all three particles (protons, neutrons, electrons) on one footing (Atkins, 1986).

Following this state of affairs, several authors have claimed that molecular structure, or the relative position of the nuclei, is not something that emerges from the calculations but rather a feature that must be imposed on the calculation from the outset. They have also claimed that *ab initio* quantum mechanical calculations thus fail to distinguish between isomers of a particular molecule such as di-methyl ether and ethanol. Both molecules consist of  $C_2H_6O$  but they have different structures ( $CH_3OCH_3$  and  $C_2H_5OH$ ). Some of these same authors claim that there are major philosophical implications such as the failure of ontological reduction of chemistry to quantum mechanics because it appears that molecular structure does not reduce to quantum mechanics. It is this train of thought that Hendry is supporting and wanting to capitalize upon in his own articles.

First let me make a general objection by saying that a similar situation applies to atoms. In trying to calculate the configuration of any atom, one needs to first assume a basis set of orbitals and to carry out a minimization of energy, then perhaps resorting to another basis set etc. This is how the configuration, or loosely speaking the structure, of any atom is arrived at. Does this signal downward causation and emergence at the atomic level? It seems that Hendry might be committed to answering in the positive and

yet this case does not depend in any way on the Born-Oppenheimer approximation.

A second immediate objection lies in asking why one should suppose that the failure of present-day quantum mechanics to determine molecular structure in an *ab initio* manner is a reflection of the ontological situation rather than just a theoretical limitation. Hendry also places the Born-Oppenheimer question into the wider context of symmetry breaking. Whereas the equations of quantum chemistry treat a molecule such as HCl as though it were symmetrical, all the properties of the molecule, such as its having a non-zero electric dipole, point to its being asymmetrical.<sup>7</sup> How does this broken symmetry come about?

According to Robin Hendry this mysterious symmetry breaking should be identified with downward causation. This amounts to the claim that symmetry breaking ‘comes from above’, as it were, and tells the molecule what structure to adopt. But again, how can one be sure that this symmetry breaking is an ontological feature? Could it not be that molecular quantum mechanics in its present state of development is still not able to capture structure for whatever reason? Structure, the chemist would argue, is surely present right from the start, whatever the equations seem to imply according to the present state of theoretical development.

Hendry then provides a possible counter-argument that would render emergence and downward causation unnecessary but is quick to dismiss it.

The symmetry problem arises in the first instance by considering the Schrödinger equation for an isolated molecule, and the only obvious solution is to appeal to the molecule’s interaction with its environment, which would be represented by a symmetry-breaking non-Coulomb term in the molecule’s Schrödinger equation. The particular form of the symmetry-breaking addition must be justified however, and it is quite mysterious how that could work if all one has in the environment are more molecules described by Coulombic Hamiltonians (Hendry, 2010, p. 186).

What Hendry has perhaps alluded to, without specifically mentioning it, or maybe unwittingly, is the subject of quantum decoherence, a mechanism that is increasingly discussed by theoretical physicists (Joos, 2006; Zurek, 1991). For many years it seemed rather mysterious that quantum states are represented by a superposition whereas we do not see superpositions in the macroscopic world. The Schrödinger’s cat paradox continued to puzzle physicist. How does the mere act of observation cause

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<sup>7</sup> The expectation value for the dipole moment of a molecule in an arbitrary eigenstate of the full molecular Hamiltonian must be zero.

the superposition of the dead and live cat to collapse into a cat that is either dead or alive but not both at once?

Then sometime around the 1970s a novel view began to emerge, under the name of “decoherence”. According to this idea the collapse of the wavefunction does not occur instantaneously but takes a certain amount of time that can be calculated depending on the system in question. And the collapse no longer has to come about as a result of observation as such. The place of observation is taken by the environment. One no longer has to be concerned about whether somebody is “watching a tree falling in the forest in order for there to be a sound”. It is no longer believed that observation is essential for there to be a collapse of the wavefunction or, in other words, for there to be a change from a coherent superposition of states to a situation in which this coherence is lost to produce specific outcomes.

And the environment can include anything from dust particles to the walls of the container in which the quantum system is present. It turns out that true coherence only exists in an isolated system.<sup>8</sup> Any system that interacts with its environment suffers a loss of coherence. The question then becomes one of the time which is required for such a decoherence process to take place.

Consider for example the case of di-methyl ether and ethanol. As stated above, both molecules consist of  $C_2H_6O$  but they have different structures ( $CH_3OCH_3$  and  $C_2H_5OH$ ). According to the quantum mechanical description the molecules of this compound exist in a superposition of both isomers or both structures. This may well be so in principle but after a very brief period of time which has been estimated to be of the order of one femto second ( $10^{-15}$  seconds), the system actualizes into either one or other of the particular isomers.<sup>9</sup>

According to the decoherence time for this molecule we see that, for all intents and purposes, the much discussed superposition of the two isomers only has a very, very transitory existence. As a result of interaction between the molecules and their environment, which includes the container that they are placed in, one or other isomer is formed. So when Hendry claims that the only environmental influence to break the symmetry would be other molecules of the compound he has neglected the

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<sup>8</sup> This point is disputed. Castagnino and Lombardi claim that quantum decoherence can also occur in open systems (Castagnino, Lombardi, 2004).

<sup>9</sup> This calculation has been carried out by my UCLA colleague Benjamin Schwartz who has published papers on quantum decoherence in the context of chemistry. R. E. Larsen, M. J. Bedard-Hearn and B. J. Schwartz (2006).

effect of other influences such as other particles or simply the walls of the container.

The concept of molecular structure therefore becomes relativized according to the time scale involved. If one considers time scales shorter than a femtosecond and a system of molecules that is completely isolated from its environment, which includes the container holding the molecules, then yes it is the case that the molecules exist in a superposition of various isomers and that 'structure' in the normal chemical sense is ambiguous. However, for all other more realistic situations encountered in chemistry and physics too for that matter, decoherence sets in very quickly and one or other structure or isomer may be said to exist.

Hendry also writes,

...if the acidic behaviour of the hydrogen chloride molecule is conferred by its asymmetry, and the asymmetry is not conferred by the molecule's physical basis according to physical laws, then surely there is a *prima facie* argument that ontological reduction fails. Of course future physics and chemistry may support ontological reduction, just as it may solve the related quantum-mechanical measurement problem, but proponents of ontological reduction are not entitled to presume that it will (Hendry, 2010, p. 187).

It would appear that current chemistry and physics has undergone a major advance whereby even if the quantum-mechanical measurement problem has not been solved outright, then it has at least been sufficiently clarified to show that for all realistic purposes, the superposition of states is of no consequence whatsoever. It's just that prior to the recent work on decoherence there had been no way in which to quantify just how serious this problem was and it had been assumed that it was all pervasive.

Moreover, one must question Hendry's suggestion that the onus lies with the reductionist to show that emergence does *not* take place or that ontological reduction does *not* fail. Surely the onus lies rather with authors such as Hendry, who propose such exotic effects as emergence and downward causation, which are not generally accepted, to argue *for* their existence.

But Hendry follows his claim by what seems to be a non sequitur when saying,

...but there is no particular reason to think the successor to quantum mechanics will exclude downward causation. In fact the inductive evidence is that it will not, because its immediate predecessor, quantum mechanics, does not (Hendry, 2010, p.187).

This claim depends on the rather dubious view of Hendry's that present day quantum mechanics does not exclude downward causation. I suspect that this claim is not shared by many researchers in the field of the foundations of quantum mechanics. If it is a widely shared view, it behooves Hendry to cite such experts in the field.

Overall, I think that Hendry has failed to heed his own warning that any ontological conclusions that one draws about reduction and emergence must be free of considerations having to do with the current state of scientific knowledge since the main thrust of his proposal lies with the current interpretation of the Born-Oppenheimer approximation or rather with an interpretation that fails to take into account recent views on quantum decoherence.

Finally, I personally remain agnostic about the existence of emergence and downward causation. Certainly the arguments put forward by Robin Hendry concerning molecular structure do not cause me to become a convert to emergence and downward causation.

## Conclusion

I believe that the philosophy of chemistry in its many and diverse forms is alive and well. The new discipline is being practiced all over the world and I note in passing that there appears to be a special interest in some Latin American countries. I am referring especially to Argentina and Brazil, Chile, Colombia and Mexico, the ones that I am personally aware of. The reason for this state of affairs is not altogether clear but may-well be due to the fact that the subject of philosophy of science or 'epistemology' is introduced in secondary level general education.

The articles in the current volume attest to the depth and breadth of the study of foundational aspects of chemistry in many nations and by specialists in many areas such as chemistry, physics, education, history, philosophy and sociology. No doubt the field will benefit greatly from the publication of the present book that succeeds in bringing together authors who do not generally attend the same meetings, and who might not be aware of each other's work. Finally, and in order to stimulate further discussion, I might also mention the appearance of a recent article on the philosophy of chemistry in the prestigious on-line *Stanford Encyclopedia of Philosophy*<sup>10</sup> and a published reaction to this approach to doing philosophy of chemistry (Scerri, 2011).

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<sup>10</sup> R. Hendry, P. Needham, M. Weisberg,  
<http://plato.stanford.edu/entries/chemistry/>

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# THE CHEMICAL BOND: SOME HISTORICAL INSIGHTS

KOSTAS GAVROGLU AND ANA SIMÕES

So to the question: has the chemical bond now done its job? Have we grown to that degree of knowledge and that power of calculation that we do not need it? ...This a tantalizing question. And only a little can be said by way of comment. Chemistry is concerned to explain, to give us insight, and a sense of understanding. Its concepts operate at an appropriate depth, and are designed for the kind of explanation required and given. If the level of enquiry deepens, as a result of our better understanding, then some of the older concepts no longer keep their relevance. (...) From its very nature a bond is a statement about two electrons, so that if the behaviour of these two electrons is significantly dependent upon, or correlated with, other electrons, our idea of a bond separate from, and independent of, other bonds must be modified. In the beautiful density diagrams of today the simple bond has got lost. It is as if we had outgrown the early clothes in which, as children, we could be dressed, and now needed something bigger. But whether that ‘something bigger’ that should replace the chemical bond, will come to us or not is a subject, not for this Symposium, but for another one to be held in another 50 years time, and bearing for its title: the changing role of chemical theory.<sup>1</sup>

## Introduction

In 1969 in a symposium on the “Fifty Years of Valence”, using his typically elegant wording, Charles Alfred Coulson, the quantum chemist, author of the well-known textbook titled *Valence* (1960), and Professor of Applied Mathematics at the University of Oxford, mused over the evolving nature of concepts and their role in fulfilling the explanatory function of scientific disciplines. He selected the chemical bond as the kernel of his musings. For him, as for many others, among chemical concepts the chemical bond reigned supreme. Its changing meanings and various visual representations had their beginnings on the old notion of

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<sup>1</sup> Coulson (1970, p. 287).

chemical affinity of Newtonian origins. They were, further, modified by the suggestion that affinity was the result of attractions of opposite (negative and positive) electrical charges, which was an approach that more or less dominated classical structural chemistry and valence theory in the second half of the 19<sup>th</sup> century. The (notion) of the chemical bond was radically rearticulated within the realm of quantum chemistry, starting in the late 1920s, with the contributions of such luminaries as Walter Heitler, Fritz London, Linus Pauling, Robert Sanderson Mulliken, Coulson, Raymond Daudel, Per-Olov Löwdin and many more.

In the quote above, Coulson refers vaguely to changes in the conception of bonds, by pointing to the correlation between level of inquiry, explanatory power and conceptual refinements. He also refers implicitly to G.N. Lewis' suggestion of the pairing of electrons as the precursor to covalent bonds, which found a quantum mechanical justification in the 1927 joint paper of Heitler and London. Furthermore, he points out to quantum mechanical calculational refinements introduced by the consideration of electronic correlations, and ends with a reference to the visualizations associated with density diagrams, whose role in quantum chemistry was increasingly important, as computers were becoming the long sought for company of every theoretical chemist.

But even the quantum mechanics era of the chemical bond, has not been a smooth period. It was the result of many contributions, the most relevant of which we briefly summarize in what follows. Lewis's suggestion of the pairing of electrons as the substratum for covalent bonds, literally inventing a quantum effect with classical entities; its quantum mechanical underpinning by Heitler and London in their groundbreaking 1927 paper, and their ulterior unsuccessful exploration of the characteristics of valence in the framework of group theory; the parallel, but independent, proposal of Erich Hückel of a quantum mechanical explanation of double bonds and of aromatic properties by taking seriously the non-visualizable constraints imposed by quantum mechanics; Pauling's introduction of rules informed by a mixing of quantum mechanical principles and empirical evidence to explain the tetra-valence of carbon by means of the novel concept of hybridized orbitals, succeeded by the explanation of bond characteristics in benzene-like molecules by recourse to the introduction of the concept of resonance among valence structures, together with his extension of the notion of chemical bonds in order to accommodate bonds made up of an uneven number of electrons (one- and three-electron bonds), all imbedded in a potent move to give a new life to structural chemistry; Mulliken's radical, but initially qualitative, proposal, based on the extension of Bohr's building-up

principle from atoms to molecules, then on Hund's work on stationary states in quantum mechanics, backed up by spectroscopic analysis, to abandon altogether the notion of atoms as the necessary substratum of molecules, and to eradicate simultaneously from chemical theory the notion of bonds as the means to glue atoms together; Coulson's appropriation of Mulliken's molecular orbital approach, endowing it with an increasingly sophisticated degree of mathematization, extending it to polyatomic molecules, and explaining mathematically such notions as fractional bonds and orders, and other characteristics of the electronic structure of molecules, together with the concomitant appropriation of one of the most appealing building blocks of Pauling's valence bond approach, that is, its amenability to pictorial representations, which was to found an extended application with the systematic use of electronic digital computers; Daudel's efforts to build a coherent framework to solve the incompatibility between quantum mechanical notions such as non-locality and quantum chemical notions such as localized bonds;<sup>2</sup> the Pullman's efforts to extend the domain of quantum chemistry to big molecules of biological interest or macro-molecules, and at the same time keeping a degree of quantitiveness, formerly associated just with smaller molecules; and, finally, Löwdin's agenda to establish quantum chemistry into secure foundations within quantum mechanics, together with the exploration of its connections with solid-state theory and material sciences.

The various epistemic aspects highlighted above enable one to identify two main parallel moves associated with the increasing degree of mathematization of explanations together with their corresponding amenability to visual representations: there was a shift from qualitative to semi-quantitative to mathematically more sophisticated explanations, at the same time that visualizability was lost and regained again, thanks to the pictorial potentialities offered by computers. But while in the former bird's eye view of disciplinary development we centered on a few individuals' conceptions of the chemical bond, one should have in mind that they often stood for different quantum chemical practices depending on different sorts of instrumentation, and frequently their apparent antagonistic features were appropriated in such a way that the constitutive characteristics of quantum chemistry stemmed more from a confluence of

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<sup>2</sup> One should note that Hund and Mulliken have also worked on this topic by means of localized and delocalized molecular orbitals labeled by Mulliken as "true MO".

diverging practices, from what we could name as a “mangle of practices,”<sup>3</sup> than from a succession of opposite trends.

Chemical lecturers and textbook writers tend to present the evolving re-conceptualizations of the chemical bond in the context of a strictly internalist narrative, often starting with classical structural chemistry, and proceeding into theoretical and quantum chemistry, and therefore concentrating usually on conceptual development and disregarding other aspects that play a relevant role in the formation of disciplines. However, it is possible to offer to those interested in the study of the history of modern chemistry a more complex and nuanced narrative in which various strands, including, but not restricted to, epistemic ones, are inextricably intertwined. In the quote above, Coulson offered a brief historical survey of major steps associated with the successive meanings of chemical bonds, in the framework of philosophical considerations on the changing role of chemical theories. In what follows, we first propose to narrate the development of an “in-between” discipline such as quantum chemistry through six interrelated clusters of issues that manifest the particularities of quantum chemistry along its evolving (re)articulations with chemistry, physics, mathematics and biology, as well as its institutional positioning. Then, we illustrate how one such issue—the emergence of computers— informed subsequent discussions on the future role of the chemical bond in the framework of quantum chemistry.<sup>4</sup>

## 1. Another Look at the History of Quantum Chemistry

Our cluster of interrelated issues includes epistemic aspects, issues related with disciplinary emergence, the re-articulation of the practices of quantum chemists brought about by the electronic computer, as well as matters related to philosophy of science, and to styles of reasoning, and, finally, the awareness of the contingent character of quantum chemistry.

The first cluster involves issues related to the historical becoming of epistemic aspects of quantum chemistry: that is, the multiple contexts which prepared the ground for its appearance, the ever present dilemmas of the initial practitioners as to the “most” appropriate course to choose between the rigorous mathematical treatment, its dead ends, and the semi-empirical approaches with their many promises, the novel concepts introduced and the intricate processes of their legitimization. Quantum

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<sup>3</sup> Pickering (1995).

<sup>4</sup> In this paper we introduce ideas that are developed more fully in our book. (Gavroglu & Simões, 2011).

chemistry appears to have been formed through the confluence of a number of distinct trends, with each one of them claiming to have been the decisive factor in the formation of this discipline: neither the relatively straightforward quantum mechanical calculations of London and Heitler in 1927, nor the rules proposed by Mulliken to set an *Aufbau* principle for molecules, nor Pauling's reappropriation of structural chemistry within a quantum mechanical context, nor Coulson's and Hartree's systematic, but at times cumbersome, numerical approximations, could be said to have given quantum chemistry its epistemic content and institutional framework. The becoming of quantum chemistry has been the result of an attitude by many physicists, chemists, mathematicians, biologists and computer experts who did not feel constrained by any of these approaches so that to be discouraged from investigating the multitude of possibilities provided by the many alternatives. Though it may appear that there is a consensus that quantum chemistry had always been a "branch" of chemistry, this was not so during its history, and different scientific communities such as physicists and applied mathematicians attempted unsuccessfully to appropriate it differently.

The second cluster of issues is related to disciplinary emergence. The naming of chairs, university politics, textbooks, meetings, networking, as well as the alliances quantum chemists sought to establish with practitioners of other disciplines, became quite decisive in the formation of the character of quantum chemistry. The emergence of quantum chemistry in the institutional settings of Germany, the USA and the UK, and later on in France and Sweden, and a number of conferences and meetings of a programmatic character, helped to mould its character. A marginal activity at the beginning, it had the good luck to have gifted propagandists and able negotiators among its practitioners. Heitler's, London's and Friedrich Hund's rather ascetic yet strong pleas for forcing chemical problems into the rigorous mathematical treatment behind the first principles of quantum mechanics; Mulliken's tirelessness in familiarizing physicists and chemists with the attractiveness of the molecular orbital approach; Pauling's aggressiveness to push resonance theory as the only way to do quantum chemistry; Coulson's incessant attempts to popularize his views in order to explain the character of valence; Daudel's and Pullmans' researches into molecules with biological interest; and Löwdin's founding of a new journal, all these, contributed towards the gradual formation of the characteristics of the emerging subdiscipline.

The third cluster of issues is related with a rather unique development in the history of this subdiscipline: the re-articulation of the practices of the community after the early 1960s that was brought about by a single

instrument—the electronic computer. The fundamental disadvantage of quantum chemistry, that is, the impossibility to perform analytical calculations, was, all of a sudden, turned into an invaluable advantage for the further legitimization of electronic computers. In the early days of computers it appeared that a whole subject depended on this particular instrument in order to produce trustworthy results. And, progressively, ever more scientists started to realize that “quantum chemistry is no longer simply a curiosity but is contributing to the mainstream of chemistry.”<sup>5</sup> The prospect of *ab initio* calculations, which did not use experimental data built in the equations in any way, seemed to offer the promise of new and reliable results, and soon reached a sophistication and accuracy to serve the needs of each quantum chemist. The members of a whole disciplinary community, through a historically complicated process had attained a consensus about the coexistence of two approaches — the valence bond method and the molecular orbital approach. In a few years they became subservient to the limitless possibilities of computations provided by a particular instrument. By then, most of the leaders of the different traditions were nearing the end of their careers, since they had all gotten into quantum chemistry when they were very young. Fostered by the use of computers, applied to *ab initio* but also to semi-empirical calculations, members of the quantum chemical community recognized that a new culture of doing quantum chemistry was asserting itself and was carving a dominant place among the more traditional ones. It was identified by a novel style of scientific thinking, in which the increasing complexity of molecular problems was dealt with by means of mathematical modeling, and a burst of activities in relation to the writing and dissemination of computer programs. Eventually, it, even, became unnecessary to perform expensive experiments, since calculations would provide the required data!

The fourth cluster of issues is related to a hitherto totally neglected aspect of quantum chemistry, that is, its contingent character. Quantum chemistry could have developed differently, and it is straightforward to show that the particular form it took was historically situated, at times being the result of not only technical but also of cultural and philosophical considerations. The historiographic possibilities provided by the category of contingency for the development of the natural sciences have been intensely discussed among historians and philosophers of science. The elaboration of this issue is not in order to make partisan points, but in

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<sup>5</sup> N/A “Computational Support for Theoretical Chemistry”. (1971), p. 1.

order to argue that, perhaps, “in-between” (sub)disciplines provide a privileged context in order to investigate the interpretative possibilities provided by the notion of contingency. Contingency is not an invitation to do hypothetical history. It is not an invitation to ruminate about meaningless “what if” situations, but rather to realize that at every juncture of its development, quantum chemistry had a number of ways along which it could have developed. What is important to understand is not what different forms quantum chemistry could or might have taken, but, rather, the different possibilities open for developments and the set of accommodations, difficulties and resistances that at each particular historical juncture formed those human and non-human barriers that dissuaded practitioners from pursuing these possibilities. Throughout its first fifty years, the criteria for assessing the “appropriateness” of the schema being developed gravitated between a rigorous commitment to quantum mechanics, a pledge towards the development of a theoretical framework where quasi-empirical outlooks played a rather decisive role in theory building, or a vow to develop approximate techniques for dealing with the equations.<sup>6</sup> Such criteria were not, strictly speaking, solely of technical character, and the choices adopted by the various practitioners at different times, had been conditioned by the methodological, philosophical and ontological commitments as well as institutional considerations, local resources and research practices. It is only through such an analysis that we can understand the idiosyncratic culture of quantum chemistry as an entangled cluster of evolving technoscientific networks.

The fifth cluster of issues is related to philosophy of science. It is undoubtedly the case that in recent years there has been an upsurge of scholarship in the philosophy of chemistry, and understandably quantum chemistry has played a prominent role in such a new situation due to the prominent and, at times excessive role played by reduction. It is also the case that a number of papers and discussions have had as their starting point issues that have been all too common in the history of quantum chemistry. We have in mind issues such as reductionism, scientific realism, the role of theory, including its descriptive or predictive character, the role of pictorial representations and mathematics, the role of semi-empirical versus *ab initio* approaches, the status of theoretical entities and of empirical observations. The successes of quantum mechanics in chemistry induced many to bring to the fore a number of philosophical issues about chemistry, or to discuss problems other philosophers of

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<sup>6</sup> It is currently the same when Truhlar and Adamo, to quote but them, shape new functionals of density (DFT) to describe molecular geometry or height barriers.

science had been discussing, but, now, within the context of chemistry. Reductionism turned out to be one of the pivotal issues. Philosophers of chemistry could certainly use these instances to re-address issues from the perspective of emergence, pointing to a re-consideration of main guidelines in the philosophy of science.

The sixth cluster is of a quasi-methodological and quasi-cultural character. The history of quantum chemistry displays instances that can be further understood in terms of “styles of reasoning”. Such an approach can tell us how decisive the “style” of a researcher was for discovering new phenomena, developing effective methods or proposing novel explanatory schemata.<sup>7</sup> A style of thought brings into being candidates for truth. The types of styles are introduced as categories of possibilities, the range of possibilities depending upon that style.

The various developments in quantum chemistry help us to provide some answers to questions like: how can styles be differentiated from one another? Is the difference in styles merely an expression of personal idiosyncrasies? Is one justified to even talk about different styles of scientific inquiry when discussing the physical sciences, since the “objective” nature of what is being investigated seems to point to a methodological uniformity? Is it at all meaningful to compare two different types of discourse? And, if it is, how are those differences to be expressed? A style possesses a peculiarly self-referential character about the criteria it sets, and against which it assesses its own coherence. What Heitler and London did by using group theory in the study of valence, what Mulliken proposed by extending Bohr's *Aufbau* principle to molecules, and proceeding into the articulation of molecular orbitals, and what Pauling did with his resonance theory, all these, can also be considered as alternative styles.<sup>8</sup>

We suggest that these six axes—the epistemic content of quantum chemistry, the social issues involved in disciplinary emergence, the contingent character of its various developments, the dramatic changes brought about by the digital computers, the philosophical issues related to the work of almost all the protagonists, and the importance of styles of reasoning in assessing different approaches to quantum chemistry—form the narrative strands of the history of quantum chemistry. And we venture to further propose that they may be a useful way to deal with the becoming of other “in-between” sub-disciplines. It is, however, certainly the case

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<sup>7</sup> Hacking (1985, p. 145-165).

<sup>8</sup> The same can be said of the work of current quantum chemists such as Bader, Truhlar, Grimme and others in the framework of DFT, ELF, AIM and metadynamics approaches.



that they appear to be indispensable for understanding how quantum chemistry developed during its first fifty years.

## 2. Computers and the Chemical Bond

The introduction of computers into quantum chemistry, by offering the prospect of unlimited computations, changed radically the face of quantum chemistry. While disciplinary identity was initially built by circumventing the obstacle of exact computations, the potentialities of computers forced the discipline to rethink its former practices and to reassess the joint role played by chemical concepts, input from experiments, increasing mathematization and function of visualizations in discipline building. Therefore, it is no surprise that the period during which the use of computers became practical, turned out to be the period during which chemists were forced to rethink the status of the chemical bond. In the quotation at the beginning of this paper—as well as in the views expressed in the after-dinner speech of the 1959 Boulder Conference—computers and practical computing lay behind Coulson's radical suggestion that the chemical bond might be irretrievably lost, despite his hope to the contrary.

What makes the Boulder Conference an event with a particular interest for historians of science was that it marked, in no uncertain terms, the transition from the founding generation of quantum chemists to a generation whose success would be dependent on the way they would make use of the electronic computers. During the Conference the promising prospects of the electronic computers were discussed together with the dangers these prospects could bring to the character of quantum chemistry as it had been articulated since the Heitler-London 1927 paper. Everyone was convinced that improving the calculational techniques and electronic hardware brought forth many and new results. But not everyone agreed on the extent to which the new practices distorted accepted norms and changed the representations quantum chemists held of their identity, thus reconfiguring quantum chemistry (almost) beyond recognition.

Perhaps Bernard Ransil—one of Mulliken's close young collaborators at his Laboratory of Molecular Structure and Spectra in Chicago—was the person who better captured the “climate” of the meeting. He conceded that the digital computer could provide the framework for “justifying” the use of a number of concepts and become an indispensable aid to turn structural chemistry into “less of an art and more of a science.” But its extensive and indiscriminate use could “blunt one's critical faculties and stunt the free play of his scientific imagination,” reducing disastrously the practice of quantum chemists to little more than calculations for the sake of

calculations. Following Mulliken's assessment, his opinion was that a middle ground existed "where the digital computer, intelligently used as a research instrument, can quickly provide the theoretical chemists with accurate results to an illuminating but complex critical calculation. Properly used, the numerical experiment can be as much of an aid and stimulus to the theoretical chemist as a well thought out and executed physical experiment."<sup>9</sup>

As it is clear from this initial statement, Ransil quotes views without acknowledging the sources, so that we can surmise that these views were widely circulating and were, in fact, characteristic of the shop talk of the community. These views expressed the core of a wide spectrum of opinions, which were no doubt expressed in the soul-searching discussions during the conference. Interestingly, he did not uncritically embrace all promises of a golden future. But he emphasized that a number of household words for the quantum chemist such as bond order, bond length, charge density, conjugation, hyperconjugation, and resonance would "benefit from a reevaluation based upon accurate *a priori* quantum mechanical calculations."<sup>10</sup>

Coulson was, we think, the protagonist of the Conference, trying to balance the worries of a generation that had established quantum chemistry and the aspirations of the younger practitioners. Despite his own contributions and those of his research associates to the calculation of molecular integrals using ever more elaborate computer programs, Coulson was never oblivious of the major shortcomings of their indiscriminate use and abuse. At the end of the 1950s he started realizing that deep changes had occurred within the community of quantum chemists, partly because members of the new generation were not anymore "middlemen" between theory and experiment as the first generation of quantum chemists were. They did not share Pauling's practical knowledge in the domain of crystallography nor Mulliken's expertise in spectroscopy, for instance.

Coulson delivered the after-dinner speech, summing the main trends of the meeting and listing the problems he felt were to occupy the chemists in the years to come.<sup>11</sup> He realized that there are now deep and perhaps irreconcilable divisions in the community of quantum chemists. These are divisions that he felt are absolutely detrimental to the discipline. The splitting, he thought, in the community resulted from the antagonism of two extreme groups. Group I possessed great computational skills and

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<sup>9</sup> Ransil (1960, p. 239).

<sup>10</sup> Ibid.

<sup>11</sup> Coulson (1960).

advocated that there are a number of problems that a dispute can only settle by computation since experiments are too difficult. To many people, this group of chemists appeared to be moving away from the conventional concepts of chemistry, such as chemical bonds, orbitals and overlapping hybrids “as to carry the work itself out of the sphere of real quantum chemistry.”<sup>12</sup> On the other extreme, Group II privileged calculations with very rough approximations for biological molecules. These calculations give quite interesting results but the approximations put forward would be greatly upsetting to the people who used extensively computers.

Coulson thought that it would be an oversimplification to think that the difference is only a difference having to do with the use of electronic computers. It was certainly the result of different ontological and epistemological allegiances. In their desire for complete accuracy, Group I appeared to be prepared to “abandon all conventional chemical concepts and simple pictorial quality in their results.” Against this, the exponents of Group II argued that chemistry is an experimental subject, whose results are built into a pattern around quite elementary concepts. He did not make any effort to conceal that his sympathies lay with the latter, and re-emphasized that the role of quantum chemistry is to understand these concepts, and to reveal the essential features in chemical behavior. Nevertheless, he was also aware that none of these concepts could be made rigorous. Coulson’s attitude at the Boulder Conference has to be seen under the background of his former concerns over the role of concepts in discipline building, bearing in mind that he and his group were also among those who initially favoured a more mathematical grounding for quantum chemistry, and who fostered the exploration of many numerical applications, soon to be succeeded by computational ones.

He wizzily fought for the cohabitation of valence bond theory and molecular orbital theory, explored sound mathematical expressions for many empirical characteristics of chemical bonds, reintroducing pictorial representations as crucial components of quantum chemical theory. He acted as a skilled go-between trying to sustain the discussions and common concerns between peers, different scientific communities and various academic environments. He also excelled as a go-between involving a new generation of practitioners, whom he trained in the discipline by writing for them a most needed textbook offering new vistas into the chemical bond. At the same time, his work and, especially, his *Valence*, was heralding the first permanent dents to Pauling’s dominant edifice.

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<sup>12</sup> Ibid.

The importance bestowed on the clarification of the *natures*—not really the *nature*, as Pauling stubbornly assumed—of the chemical bond is evident when we realize that the two first landmark textbooks of the discipline were precisely titled *The Nature of the Chemical Bond* and *Valence*, and therefore centred on the appropriation of old conceptions of bonds into quantum chemistry, followed by the exploration of their new meanings.

Along the way, Coulson had been discussing the status of concepts in chemistry and especially the status of the chemical bond. For Coulson, the chemical bond was a “concept of the imagination” endowed with strong heuristic power. He kept on reminding his audience that all chemistry rests on the idea of a chemical bond, and every generation of chemists has tried, in its own way, to describe what a bond is. The different descriptions that have been given show how greatly our understanding of the “real essence of chemistry” has developed in the past since Frankland or Kekulé.<sup>13</sup> For nearly one hundred years chemists noticed the characteristic affinities of one substance for another. Lewis had suggested that this affinity is related to the disposition of two electrons, but “remember, no one has ever seen an electron!”<sup>14</sup> The quantum mechanical underpinning of Lewis’s description showed that the shared electrons have their spins pointing in opposite, or anti-parallel, directions, but “remember, no one can ever measure the spin of a particular electron!”<sup>15</sup> However, everyone was captivated by “the simplicity of the idea.”<sup>16</sup> Then the distribution in space of these electrons is described analytically with closer and closer degrees of precision, but “remember, there is no way of distinguishing experimentally the density distribution of one electron from another!”<sup>17</sup>

In the meantime, concepts like hybridization, covalent and ionic structures, resonance, and fractional bond orders had been introduced as ad-hoc assumptions. Coulson was rather uneasy that none of these concepts could be linked to a directly measurable quantity. Nevertheless, “chemical knowledge and, perhaps even more, chemical intuition, find their full expression and their proper setting within the mathematical framework that has now been devised.”<sup>18</sup> The importance of conceptual insightfulness together with the usefulness and truthfulness of concepts is stressed again and again in Coulson’s writings. He felt that a bond is “no

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<sup>13</sup> Coulson (1952, p. 11).

<sup>14</sup> Coulson (1953, p. 20-21).

<sup>15</sup> Coulson (1953, p. 20-21).

<sup>16</sup> Coulson (1970, p. 287).

<sup>17</sup> Coulson (1953, p. 20-21).

<sup>18</sup> Coulson (1952, p. 13).

more real than the square root of  $-1$ !”<sup>19</sup> And he continued to hold this view a couple of years later when he noted that:

Sometimes it seems to me that a bond between two atoms has become so real, so tangible, so friendly that I can almost see it. And then I awake with a little shock: for a chemical bond is not a real thing: it does not exist: no-one has ever seen it, no-one ever can. It is a figment of our own imagination.<sup>20</sup>

What was going to happen in the future to the idea of a bond? Coulson gave two possible answers to this interesting question. The work of the following years will have to be more concerned with refining, and perhaps simplifying, the sort of description already worked out.<sup>21</sup> But in the quote, dated from 1970, with which we began this paper, Coulson was already distancing himself from the worries voiced at the Boulder Conference, already a decade in the past. He could now pause to offer a more radical possibility: the chemical bond will be lost and “something bigger” should come to replace it. He conceded so much importance to the debate of such topics that he ventured to propose that in fifty years time, another symposium should be dedicated to “the changing role of chemical theory.”<sup>22</sup> If that conference is ever going to take place is still to be seen. Yet, if history is to provide us with any clues at all, we may expect that the concept itself will continue to be going through various metamorphoses.<sup>23</sup>

## Concluding Remarks

Whether chemistry, and chemical concepts such as the chemical bond, had been forgotten in the euphoria of the age of the computer is a debatable issue. What, however, is not debatable is that from the very beginning of the period when chemical problems were examined quantum mechanically, everyone involved in the subsequent developments tried to understand the character of what resulted from the encounter(s) of chemistry with quantum mechanics.

Perhaps it may be argued that the involvement of almost all those who did pioneering work in quantum chemistry in the various discussions and disputes—either in their published papers or in their correspondence or in

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<sup>19</sup> Coulson (1953, p. 20-21).

<sup>20</sup> Coulson (1955, p. 2084).

<sup>21</sup> Coulson (1952, p. 12).

<sup>22</sup> Coulson (1970, p. 287).

<sup>23</sup> That is really the case in the latest chemical quantum approaches of reactivity.

their public lectures—had to do with *legitimizing the epistemological status of various concepts in order to be able to articulate the characteristic discourse of quantum chemistry*. Legitimizing a discipline, however, is not only related to the clarification of the content of the proposed concepts and the correctness of certain approaches and practices. The process itself is a rigorously social process, involving rhetorical strategies, professional alliances, institutional affirmations, presence in key journals and conferences.<sup>24</sup>

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<sup>24</sup> The authors thank Jean-Pierre Llored for his perceptive comments and suggestions.

# THE RELEVANCE OF BOYLE'S CHEMICAL PHILOSOPHY FOR CONTEMPORARY PHILOSOPHY OF CHEMISTRY

MARINA PAOLA BANCHETTI-ROBINO

There are more things in heaven and earth, Horatio,  
Than are dreamt of in your philosophy.

—*Hamlet*, Act 1, scene 5

## Introduction

Much of 20<sup>th</sup> century philosophy of science focused its attention primarily on physics and on the fundamental philosophical issues raised by its methods, principles, and theories. As a result of this emphasis on physics, many of the other sciences were either ignored or claimed to be “derivative” sciences that raised no unique or peculiar philosophical concerns of their own. For positivistic philosophy of science, the so-called “derivative” sciences were ontologically and epistemologically reducible, without remainder, to the fundamental science of physics. Thus, all philosophical questions that could be raised with regard to these “derivative” sciences were believed to be entirely reducible to philosophical questions in physics. As positivism in the philosophy of science began to wane, however, greater philosophical interest arose in chemistry, biology, and other sciences so that, by the end of the 20<sup>th</sup> century, the philosophies of chemistry, of biology, and of other sciences began to be recognized as legitimate subfields within the philosophy of science, although the global acknowledgment of these subfields is still weak.

The philosophy of chemistry is, therefore, a relatively new subfield of contemporary philosophy of science. What I hope to demonstrate in this essay, however, is that the issues that it raises are not new to contemporary philosophy of chemistry but were already pondered by chemists in the early stages of modern chemistry. In particular, I wish to show that Robert Boyle, one of the founding figures of modern chemistry, not only

anticipated many of the fundamental problems that inform philosophy of chemistry today but also developed a chemical philosophy to address these philosophical concerns in a manner compatible with the results of his experimental work. Ultimately, I hope to demonstrate that, unlike contemporary philosophers of science who did not recognize the philosophical import of chemistry until recently, early modern chemists such as Robert Boyle were quite certain that chemistry raises some serious philosophical concerns of its own that are not merely reducible to philosophical questions in physics. This is due in part to the fact that, for Boyle, chemistry was not at all a “derivative” science, as positivists would have it, but an autonomous science irreducible to and independent from physics.

To achieve my task, I will first address some of the fundamental issues in contemporary philosophy of chemistry, that is, the reduction of chemistry to physics, the emergence and supervenience of chemical properties, and the autonomy of chemical explanations and of chemistry as a science, focusing particularly on the positions taken on these issues by leading philosophers of chemistry. After this, I will discuss in detail the chemical philosophy of Robert Boyle, the fundamental philosophical issues that he encountered while doing his experimental work, and the chemical philosophy that he developed to reconcile his philosophical concerns with the findings of his experimental work.

### **Fundamental issues in contemporary philosophy of chemistry**

One of the fundamental questions in contemporary philosophy of chemistry is that of the autonomy of chemistry as a science, an issue directly related to the reduction of chemistry to physics. In fact, the issue of the reduction of chemistry to physics has been called “one of the main areas in which philosophical interest in chemistry should be directed”.<sup>1</sup> Since the ontological dependency of chemical properties on fundamental physical states is not at issue, the sort of reduction meant here is epistemic, rather than ontological, and the question is “whether our current description of chemistry can be reduced to our most fundamental current description of physics, namely quantum mechanics—and with its explanatory consequences”.<sup>2</sup> Some philosophers of science are firmly convinced that such an epistemic and explanatory reduction is both desirable and, at least

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<sup>1</sup> Scerri and McIntyre, “The case for the philosophy of chemistry”, 214.

<sup>2</sup> Ibid., 215.



in principle, achievable. Although he does not himself embrace such reductionism, Jeffery Ramsey explains that "philosophers rarely dissent from the claim that chemistry reduces to physics ... Authors acknowledge *practical* limitations to the reduction, since 'actually constructing the quantum mechanical explanations of chemical phenomena is generally beyond human capabilities' ... Nearly everyone agrees, however, that the reduction holds in principle".<sup>3</sup> Some philosophers of science go even further than to advocate reductionism in principle. They actually hold that the epistemic reduction of chemistry to physics has, in some cases, already been achieved. Hilary Putnam and Paul Oppenheim, for example, have famously claimed that it has "been possible to micro-reduce to the atomic and in some cases directly to the subatomic level most of the *macro-physical* aspects of matter ... as well as the *chemical* phenomena of the elements ... electronic theories explain, e.g., the laws governing valence, the various types of bonds, and the 'resonance' of molecules between several equivalent electronic structures ... While some molecular laws are not yet micro-reduced, there is every hope that further successes will be obtained in these respects".<sup>4</sup> Oppenheim and Putnam assume that reduction of chemistry to microphysics has already been achieved<sup>5</sup> and argue that the ability to "obtain an atom by bringing together the appropriate elementary particles"<sup>6</sup> or to synthesize molecules "by chemically uniting atoms"<sup>7</sup> is evidence that even further reduction is achievable. They claim that "whenever it *can* be shown that things of a given level existed before things of the next higher level came into existence—some degree of indirect support is provided to the particular special case of our working hypothesis [i.e., micro-reduction as an instrument for the unity of science]".<sup>8</sup> The underlying assumption in Putnam and Oppenheim's claim here is that things at the lower level are not altered by their participation in a composite at the higher level and that no new properties emerge when things at the higher level come into existence. This assumption is, of course, highly questionable and arguments against it are forthcoming in this essay.

At this time, however, let me point out that, despite this received view among many philosophers of science, chemists and philosophers of chemistry have serious doubts about whether the ontological dependency

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<sup>3</sup> Ramsey, "Molecular shape, reduction, explanation and approximate concept", 233.

<sup>4</sup> Putnam and Oppenheim, "Unity of science as a working hypothesis", 22.

<sup>5</sup> Ibid., 27.

<sup>6</sup> Ibid., 26.

<sup>7</sup> Ibid.

<sup>8</sup> Ibid., 23.

of chemistry upon physics undermines the epistemological and explanatory autonomy of chemistry as a science. The hope for such reduction, as Eric Scerri points out,

seems to have been abandoned and ... all that remains is the possibility for approximate reduction. However, criteria for approximate reduction have not been put forward and the notion remains vague ... the calculation of the ground state energies of atoms has been achieved to a remarkable degree of accuracy and similarly calculations on small or even medium sized molecules have given encouraging results. However, whether one can draw the conclusion that chemistry has been reduced rather depends on one's criteria of reduction. If we are to define approximate reduction as has been suggested ... then it must be concluded that *chemistry is not even approximately reduced to quantum mechanics* (1994: 168).<sup>9</sup>

As far back as 1939, Linus Pauling claimed that “[a] small part of the body of contributions of quantum mechanics to chemistry has been purely quantum mechanical in character; only in a few cases, for example, have results of direct chemical interest been obtained by the accurate solution of the Schrödinger wave equation ... The principal contribution of quantum mechanics to chemistry has been the suggestion of new ideas, such as the resonance of molecules among several electronic structures with an accompanying increase in stability”.<sup>10</sup> It is ironic to note that it is precisely with regard to the chemical concepts of valence and bonding, mentioned above by Putnam and Oppenheim as examples of successful attempts at reduction, that the possibility of reduction is, in fact, most in doubt. The conceptual reduction of notions such as composition and molecular structure is also in serious doubt, in part because these concepts do not represent ontological features of the world. When it comes to such concepts, reduction is just not possible even in principle “due to the very nature of the concepts themselves. That is, the concepts of composition, bonding, and molecular structure cannot be expressed except at the chemical level ... we can calculate certain molecular properties, but we cannot point to something in the mathematical expressions which can be identified with bonding. The concept of chemical bonding seems to be lost in the process of reduction”.<sup>11</sup> Hans Primas sheds doubt on the amount of insight that quantum theory can provide for understanding such chemical concepts, when he states that “many calculations have been extremely

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<sup>9</sup> Scerri, “Has chemistry been at least approximately reduced to quantum mechanics?”, 168.

<sup>10</sup> Pauling, *The Nature of the Chemical Bond*, vii.

<sup>11</sup> Scerri and McIntyre, “The case for the philosophy of chemistry”, 218-9.

sophisticated, designed by some of the foremost researchers in this field to extract a maximum of insight from quantum theory. For simple molecules, outstanding agreement between calculated and measured data has been obtained. Yet, the concept of a chemical bond could not be found anywhere in these calculations. We calculate bonding energies without ever knowing what a bond is!"<sup>12</sup>

Molecular shape also resists reduction in principle due to the fact that, according to many chemists, it is a "mere" concept, albeit one with a strong heuristic power. Although "molecular shape is a central chemical concept which has been powerfully explanatory ... Wooley, Primas, and others charge [that] shape is only a 'powerful and illuminating metaphor' ... Our traditional picture of molecules is 'a concept for solving chemical problems, not an object of belief' ... If this is correct, the fundamental idea that molecules are constructed additively of atoms, which retain their essential identity within the molecule, is brought into question".<sup>13</sup> Ramsey further explains that

[s]ince shape is widely thought to be a physical as well as a chemical attribute of the world, those who endorse the received opinion should be shocked to hear that [molecular] shape is metaphorical in virtue of being only chemical ... Molecules can lack an orientation in three-dimensional space, and a particular shape is dependent on the way the molecule is picked out in measurement. Philosophical analysis invites the idea that the question "Does  $x$  possess  $F$  or not?" is well formulated. Philosophical reasoning indicates it is not well-posed, at least for some properties. Shape is a response property rather than an intrinsic property ... essentialism about shape fails because it does not recognize the approximate nature of the concept ... Whether we need to employ the fixed nucleus picture, separate nuclear and electronic "clouds", or interacting clouds depends on the particular molecule chosen for study, the experimental technique we employ and the questions we ask. As it turns out, there are many different representations of the same response property.<sup>14</sup>

Chemical composition, a concept related to that of bonding and molecular structure, also resists reduction because "what is physical about a chemical system are its components rather than the system itself [*qua* chemical system] which possesses emergent (though explainable) properties in addition to physical properties".<sup>15</sup> This irreducibility of the chemical

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<sup>12</sup> Primas, *Chemistry, Quantum Mechanics and Reductionism*, 5.

<sup>13</sup> Ramsey, "Molecular shape, reduction, explanation and approximate concept", 233.

<sup>14</sup> *Ibid.*, 234-48.

<sup>15</sup> Bunge, "Is chemistry a branch of physics?", 210.

system to its physical components is best understood by examining the mereology of chemical systems such as molecules, for example. As Rom Harré and Jean-Pierre Llored have pointed out, “constituent atoms of molecules are not parts of those molecules when we look at the total entity in the light of molecular orbitals. Unlike chair parts which preserve their material properties whether in the chair or on the bench”.<sup>16</sup> It is also questionable whether molecules have definitive physical component parts in such a way that the concept of molecule could be reduced to the concept of physical components without remainder. Thus, Putnam and Oppenheim’s assumption that “molecules are constructed additively from atoms, which retain their essential identity within the molecule, is brought into question”.<sup>17</sup> In fact, Harré and Llored have argued that, just as there is no salt in the sea although the sea affords salt as the result of certain operations, there are no atoms in molecules although “molecules afford atoms in the context of certain manipulations as studies of molecular reactivity have shown us. The material content of a molecule can only be a fusion of atomic potentials, not of atoms [and] affordances are not simple conditional properties ... they incorporate the procedure or method used to display their empirical manifestations ... the parts of chemical wholes like molecules and atoms are affordances, not themselves concrete entities”.<sup>18</sup> This implies that the concept of a molecule can, therefore, not be reduced to the concept of constituent atoms, because these parts of the whole are not concrete entities as such and, in some cases, may be “ephemeral” individuals. For example, “the swiftly composing and decomposing hydrogen-oxygen structures of which real water is really composed are ephemeral individuals. Water is made up of these beings. As such they are [ontological] constituents of a certain whole”.<sup>19</sup> But water, as a chemical composition, cannot be simply reduced to these ephemeral parts or occurrences.

In addition to the reduction of chemistry to physics, another important and related issue in contemporary philosophy of chemistry is the question of the emergence of chemical properties from relationships at the physical level. There is, in fact, ample reason to support the notion of emergence with regard to chemical properties.

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<sup>16</sup> Harré and Llored, “Mereologies as the grammars of chemical discourses”, 11.

<sup>17</sup> Weininger, “The molecular structure conundrum: Can classical chemistry be reduced to quantum chemistry?”, 939.

<sup>18</sup> Harré and Llored, “Mereologies as the Grammars of Chemical Discourses”, 12.

<sup>19</sup> *Ibid.*, 13.

[Philip] Anderson pointed out that in general, any steady-state system configuration of matter must exhibit the same symmetries as the dynamic equations that govern it. However, while this applies to the component parts of a system in isolation, the whole might display less symmetry because of the interactions between the parts ... the phenomenon of emergence then is seen by Anderson as the demonstration of some macroscopic effect that is less symmetrical than the component parts of the system would demonstrate in isolation ... [For example] a system which has spherical symmetry, and whose state is changed because of chemical reactions and diffusion, will remain spherically symmetrical forever if the reaction and diffusion rates are identical. However, irregularities in the rates of production and diffusion of substrates result in chemical instabilities [that] break the symmetry ... the instabilities grow and form waves. The formation of a chemical wave is a form of chemical signaling. Such chemical signaling plays an important role in embryogenesis, the formation of embryo polarity (the definition of head and tail of the organism), bud and shoot formation in plants, and the structure of morphology in animals.<sup>20</sup>

When the concept of emergence is analyzed further, it is seen to involve a number of interdependent features. The first of these is novelty, that is, the component parts of a substance do not display the emergent property of that substance. The second ingredient of emergence is the metaphysical relation of supervenience, that is, "a relation of determination and dependence of one set of properties on another".<sup>21</sup> The third feature of emergence is unpredictability, which is related to the notion of

*nonsummative difference* in supervenient properties from 'subvenient' properties (that is, the supervenient properties are not, and not simply additively derivable from, those of the supervenience base. This is also intimately related to the supposed nonreducibility of the supervenient properties to the subvenient) ... The kind of mereology this calls for is quite different from the widely assumed extensional interpretation of classical mereology, in which any parts whatever automatically compose some whole, regardless of their relations to each other.<sup>22</sup>

It is important to speak of relationality in the context of a mereological account of supervenience for the following reasons. The whole that displays supervenient properties is not merely a collection of parts

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<sup>20</sup> Newth and Finnigan, "Emergence and self-organization in chemistry and biology", 845-6.

<sup>21</sup> Newman, "Chemical supervenience", 49.

<sup>22</sup> *Ibid.*, 50.

haphazardly put together but, rather, it is a composite of parts in very specific relation to one another. It is both the subvenient properties of the constituent parts and the relation of those parts and properties to one another that account for the supervenient properties of the whole, and this is what accounts for the transcendence (i.e., non-reducibility) of the supervenient properties. Because we are arguing that supervenience is a feature of emergence and because emergence is conceived as an ontological feature of the world, whereas unpredictability and derivability are epistemic notions, it is best to speak of supervenience in terms of ontological underdetermination. Following Achim Stephan, Robert Francescotti advocates replacing “the unpredictability constraint with the following underdetermination thesis: *the emergent properties of the whole are underdetermined by the properties of its proper parts ...* The crucial question [therefore] is whether the properties of the parts at one time underdetermine the properties of the whole at that same time”.<sup>23</sup>

This underdetermination is accounted for precisely through the notion of relationality. According to Joseph Earley, “[a]n adequate theory of wholes and parts (mereology) must take into account that when individuals enter combinations of interesting sorts they no longer are the very same individuals that existed prior to the composition”.<sup>24</sup> The mereology involved in chemical supervenience is a nonstandard mereology because “the parts undergo changes when they form a whole”.<sup>25</sup> The presence of the supervenient property affects the properties of the constituent parts, so that the properties of the parts are dependent upon the role that they play within the whole that expresses the supervenient property. In Earley’s words, “[m]ost philosophers have yet to recognize that, when components enter into chemical combination, those components do not, in general, maintain the same identity that they would have absent that combination”.<sup>26</sup> Good examples that illustrate Earley’s point are H<sub>2</sub>O and silver chloride. While the property of being H<sub>2</sub>O or of being silver-chloride “supervenes on features of the constituent atoms, the features of the atoms on which it supervenes include features that the atoms have only by virtue of being parts of that compound. The atomic interrelations that give rise to the compound would not obtain if the atoms were parts of a

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<sup>23</sup> Francescotti, “Emergence”, 52-3.

<sup>24</sup> Earley, “Why there is no salt in the sea”, 85.

<sup>25</sup> Newman, “Chemical supervenience”, 56.

<sup>26</sup> Earley, “Varieties of properties: An alternative distinction among qualities”, 89.

different molecular type".<sup>27</sup> Molecules themselves are defined in accordance with chemical reaction networks and not vice-versa.<sup>28</sup>

Since the emergent properties of the whole affect the properties of the constituent parts so that these parts are different than they would otherwise be, the emergent property not only displays novel causal powers but it very specifically displays downward causal influence. "To the extent that the behavior of any subsystem is affected by the supersystems in which it participates, the emergent behavior of complex systems must be viewed as determining, but not being determined by, the behavior of their constituent parts. And this is downward causation".<sup>29</sup> Thus, although supervenience is generally understood as a relationship of asymmetric dependence, so that the supervenient properties depend upon the subvenient properties but not vice versa, the sort of supervenience involved in emergence is symmetrical. The key to understanding how it is possible for a property to both supervene on the component parts and yet exert both novel and downward causal influence is, precisely, the notion of relationality explained above.

Emergence ... is a function of *relationality*. Emergent property F supervenes only given relations the parts bear to one another. Also important are relations the parts bear to the whole, since F supervenes only with the help of properties that parts would lack were they parts of a whole with F. This latter fact is what makes it possible for F to supervene and at the same time exert a *novel* and even *downward* causal influence. The influence of F supervenes on, and therefore is solely a function of, the properties of the parts. Yet the influence is novel in that it goes beyond (is not solely a function of) the properties of the parts *when taken in isolation from the whole*. And because F supervenes only with the help of properties the parts would lack were they not parts of a whole with F, the base on which F supervenes is dependent on the presence of F itself. In this way, F influences the properties of the parts without violating the supervenience relation.<sup>30</sup>

Emergence and supervenience, understood in terms of relationality and symmetrical dependence, are keys to answering the question of reducibility. Although "the phenomena we study in some secondary science are thought to be ontologically dependent upon relationships at the

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<sup>27</sup> Francescotti, "Emergence", 58

<sup>28</sup> I am grateful to Jean-Pierre Llored for suggesting this useful example.

<sup>29</sup> Hendry, "Is there downward causation in chemistry?", 180.

<sup>30</sup> Francescotti, "Emergence", 61-2.

primary level ... supervenience allows us the virtue of ontological dependence, without the vice of explanatory reduction”.<sup>31</sup>

Although Jaegwon Kim and others have argued that the concept of downward causation presents us with a paradox<sup>32</sup>, philosophers must reconcile these claims with the empirical fact that downward causation exists. As Michel Bitbol tells us, the root of the problem is not the concept of downward causation nor is the experience of downward causation but “the standard *metaphysical interpretations* that are superimposed upon them.”<sup>33</sup> Most recently, however, Bitbol has proposed an alternative way of thinking about the conceptual problem of downward causation. In fact, if we accept Bitbol’s proposal, downward causation does not present a problem at all. According to Bitbol, it is under a substantialist construal of higher and lower levels of organization that downward causation seems paradoxical. However, an alternative exists “provided the substantialist presupposition is dropped *at every single level* of description”<sup>34</sup> and a symmetric and interventionist conception of causation is adopted. The proposed conception fully embraces the quantum mechanical ideas that “observables are operationally defined and that experimental interventions are *co-constitutive*, rather than merely revealing of properties.”<sup>35</sup> Under this conception, intervention is what allows us to isolate causes so that “configuration A is a cause of the distinct configuration B if: (i) whenever A has been actively set up by any means, B occurs (with probability  $p$ ); (ii) whenever A has been actively removed, B does not occur (or occurs with probability  $p' < p$ ). Interestingly ... this definition of causality was retained by ... Galilei [who stated that] ‘The cause is that which, when posited the effect follows, and when removed the effect is removed.’ ... Several difficulties of the concepts of upward and downward causation are formally solved by this theory of causality.”<sup>36</sup> According to Bitbol, two consequences of adopting this interventionist theory of causation are that

- (i) Downward and upward causation are *neither* illusory *nor* inherently existent, but rather indexed by a certain level of intervention. Accordingly, downward and upward causation are not substantial concepts, but rather relational concepts throughout. (ii) The relevant relations do not take place between otherwise self-subsistent entities. They contribute to the very

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<sup>31</sup> Scerri and McIntyre, “The case for the philosophy of chemistry”, 224.

<sup>32</sup> See Kim, “Making sense of emergence”, 3-36.

<sup>33</sup> Bitbol, “Downward causation without foundations”, 2.

<sup>34</sup> *Ibid.*, 7.

<sup>35</sup> *Ibid.*, 10.

<sup>36</sup> *Ibid.*, 7.



*definition* of their terms ... This strongly anti-foundationalist approach does not fit well with the dominant scientific realist program of research in philosophy of science. But it makes perfectly good sense in the framework of an alternative program of research inspired by Kant's "transcendental idealism", Husserl's phenomenology, and pragmatism. After all, in this kind of framework, "the access to an object partakes of the being of this object." [Bitbol is here quoting Emmanuel Levinas, *En découvrant l'existence avec Husserl et Heidegger*. Paris: Vrin, 2001, 161]<sup>37</sup>

The issues of emergence, supervenience, and reducibility are themselves closely related to the question of the autonomy of chemical explanations and, more generally, to the question of the autonomy of chemistry from physics. The reducibility of chemical laws to physical laws would necessitate that physical laws be universal and fundamental, and that all laws in the special or secondary sciences be non-fundamental instantiations of these more general and universal physical laws. The evidence at this point, given all that has already been said about the emergence of chemical properties and irreducibility of chemical concepts, seems to weigh against the reducibility of chemical laws to the extent that at least some chemical laws can be considered fundamental.

[W]hile the mechanist posits a single fundamental law, or a few such laws, the emergentist allows that there could be a great many. Turning to chemistry in particular, the mechanist claims that just a few laws of microscopic dynamics suffice to determine the behavior of every atom or molecule ... Hence, given those few laws and the physical constitution of a chemical species, it will be possible in principle (though perhaps not in practice) to deduce a complete account of its behavior. The emergentist will allow that for some atoms and molecules, there will be fundamental laws describing only their behavior, which are not instances of more general laws.<sup>38</sup>

The nonstandard mereology discussed above can help us as we expand on the above claims. To the extent that a chemical species, understood as a whole, displays properties that are underdetermined by its component parts, the fundamental laws that govern the individual parts cannot, even in principle, permit us to deduce a complete account of the behavior of the chemical species. Furthermore, since an emergent property exerts downward causal influence on the component parts whose relations give rise to this property, and to the extent that the component parts are

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<sup>37</sup> Ibid., 2.

<sup>38</sup> Hendry, "Is there downward causation in chemistry?", 179.

therefore altered by this downward causation, the fundamental laws that govern the parts as individuals may not be the same laws that govern the parts once they exist in certain kinds of relations as parts of a whole. As Bitbol claims, “there may exist differences between global states without any corresponding differences between the local states that are supposed to underpin them ... Properties and states cannot be treated as preexistent intrinsic features. They must be construed as relational.”<sup>39</sup> As Harré and Llored have suggested, these properties may be “affordances”. It is clear from this that the few laws supposed by the mechanist to determine the physical constitution of the chemical species do not suffice to account completely (or, perhaps, even partially) for its behavior. Therefore, if fundamental physical laws do not suffice to explain the behavior of chemical species and if only uniquely chemical laws can satisfactorily provide such explanations, then one is in a position to affirm the autonomy of chemical laws and of chemistry as an independent science. As Mario Bunge claims, “even if it were possible to define every chemical concept in terms of physical concepts, and deduce every chemical law statement from a set of physical premises, chemistry would still kept is peculiar referents (chemical systems), methods (e.g., acidity measurement and neutralization), and goals (e.g. understanding and controlling chemical syntheses) ... we must regard each science as a system possessing a number of features: we must picture it as an entire field of research”.<sup>40</sup>

I now turn to the chemical philosophy of Robert Boyle, which anticipates many of the contemporary concerns discussed above and seeks to address these concerns in a manner compatible with the empirical findings of Boyle’s experimental research.

### **Fundamental issues in Robert Boyle’s chemical philosophy**

The debate over chemistry’s relation to physics is not new to contemporary philosophy of chemistry and, in fact, this debate raged on in the 17<sup>th</sup> century among many natural and speculative philosophers. As Paolo Rossi tells us, “[l]ike geology and magnetism, chemistry became a modern science between the seventeenth and eighteenth centuries”<sup>41</sup>, although a structure for it already existed in alchemy. However, for much of its history prior to the 16<sup>th</sup> century, chemistry was primarily a practical

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<sup>39</sup> Bitbol, “Downward causation without foundations”, 13.

<sup>40</sup> Bunge, “Is chemistry a branch of physics?”, 210-1.

<sup>41</sup> Rossi, *The Birth of Modern Science*, 139.

endeavor that did not seem to be anchored upon a solid theoretical and philosophical foundation. The scientific status of chemistry was, therefore, dependent upon the development of a solid chemical philosophy. "Without a doubt, *chemical philosophy* was rooted in the occult [alchemy] and its theoretical matrix was to be found in the grandiose writings of the intriguing ... Paracelsus (ca. 1493-1541). Yet *chemical philosophy* occupies an important place in the scientific culture of the seventeenth century".<sup>42</sup> As the debate over chemistry's status evolved, it was well understood by the participants in this debate that the question of scientific autonomy depended upon whether or not chemical phenomena could be reduced, without remainder, to the properties of material particles that were governed by the laws of physics. In fact, questions of ontological and epistemic reduction of chemical phenomena to fundamental physical states were widely debated issues and, to the extent that the dominant theory of matter in the 17<sup>th</sup> century was the Cartesian mechanical philosophy, supporters of reductionism argued that all chemical phenomena were reducible to the mechanistic properties of fundamental material particles, that is, to shape, size, and motion.

Although the question of the status of chemistry as an autonomous science was not raised during his time, it is safe to say that Robert Boyle would probably view chemistry as autonomous from physics, and his rejection of reductively mechanical explanations for his own experiments supports this claim. "Boyle [does] not consider chemistry as a branch of physics ... [and] Boyle [does] not reduce all chemical phenomena to the geometrico-mechanical affections of particles of inert matter".<sup>43</sup> In fact, and despite the received view among many contemporary philosophers of science, a close examination of Boyle's chemical writings shows that he distinguishes his commitment to the mechanical philosophy, which he considers the most adequate theory of matter available, from his chemical philosophy, which is solidly committed to the irreducibility of chemical phenomena. Boyle is "far from subordinating chemistry to mechanical philosophy, since he [does] not explain chemical phenomena by immediate and direct recourse to the mechanical affections of particles. As a matter of fact, he regard[s] chemistry as a discipline independent from mechanics [and explains] chemical phenomena in terms of corpuscles endowed with chemical, rather than mechanical properties. Accordingly, his chemical philosophy can be described as corpuscular, [but] not as

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<sup>42</sup> Ibid., 139-40.

<sup>43</sup> Clericuzio, *Elements, Principles and Corpuscles: A Study of Atomism and Chemistry in the Seventeenth Century*, 106.

mechanical”.<sup>44</sup> It is very clear that Boyle distances himself from those mechanistic philosophers such as Spinoza, who attempt to provide explanations for all chemical phenomena and reactions from a strictly Cartesian, mathematical, and a priori point of view, as is attested in the well-documented disagreement between Boyle and Spinoza regarding how to interpret the reintegration of potassium nitrate. Ultimately, as an experimental chemist, Boyle cannot bring himself to adopting an unrelentingly reductionist position. In fact, his disagreement with the reductionism of Spinoza and other Cartesian mechanists is obvious in *An Essay on various Degrees or Kinds of the Knowledge of natural things*, in which Boyle flatly states that Epicureans and Cartesians

are so charm'd with ye clearness & pleasure of Theorys & explications, yt are deriv'd immediately from metaphysical and mathematical notions & theorems; yet they oftentimes give forced and unnatural accounts of things, rather than not to be thought to have deriv'd them immediately from these highest principles. And, wch is much worse, they despise & perhaps too condemn or censure all yt knowledge of the works of nature yt Physicians, Chymists & others pretend to, because they cannot be clearly deduc'd from the Atoms, or ye Catholic Laws of motion.<sup>45</sup>

With regard to the aforementioned experiment, when Boyle provides an explanatory account of the reintegration of potassium nitrate, he “does not so much invoke the movement and shape of corpuscles as he does the chemical qualities of the different substances that have the properties of dissolving, precipitating, or fixing. In brief, for Boyle, chemical explanation retains its autonomy and cannot be reduced to a mechanical explanation that, without a doubt, sustains it but can never clarify it as such.” (My translation).<sup>46</sup> One can find other evidence of Boyle’s preference for chemical, rather than mechanical, explanations in the majority of his experimental accounts. In the *History of Colours*, for example, he explains his experiments with colors by relying solely on chemical properties. In one particular experiment involving Venetian sublimate (mercuric chloride), tartar of wine (potassium hydrogen tartrate), and acid spirit of vitriol (sulfuric acid), Boyle explains the change of his solution from transparent, to orange, and back to transparent as occurring due to “the

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<sup>44</sup> Clericuzio, “A redefinition of Boyle’s chemistry and corpuscular philosophy”, 563.

<sup>45</sup> Boyle, *An Essay of Various Degrees or Kinds of the Knowledge of Natural Things*, 166r.

<sup>46</sup> Joly, “Chimie et mécanisme dans la nouvelle Académie royale des sciences: les débats entre Louis Lémery et Étienne-François Geoffroy”.

substitution of compound corpuscles having chemical properties, [rather than due to] the mechanical properties of corpuscles".<sup>47</sup> Boyle justifies taking this approach on the ground that this "seems to be the Chymical reason of this Experiment, that is such a reason, as, supposing the truth of those Chymical Notions I have elsewhere I hope evinc'd, may give such an account of the *Phænomena* as Chymical Notions can supply us with; but I both here and elsewhere make use of this way of speaking, to intimate that I am sufficiently aware of the difference betwixt a Chymical Explication of a *Phænomenon*, and one that is truly Philosophical or Mechanical".<sup>48</sup> In his physiological essays, such as his *Memoirs of the History of Human Blood*, Boyle is even more explicit in giving strictly chemical explanations and altogether avoids any reference to the mechanical properties of corpuscles. As a chemist, he is strongly committed to explaining phenomena in a manner that accounts for the qualitative changes that occur in chemical operations and in "transmutations" and he is, therefore, not satisfied with reducing chemical properties to merely primary and entirely quantifiable properties of fundamental matter.

Despite his refusal to adopt a strict reductionism, it is widely accepted that Boyle embraces a Cartesian mechanistic ontology with regard to the nature of fundamental particles. The question must be raised of how Boyle can compatibly endorse both Cartesianism and anti-reductionism. In order to answer this question, one must understand Boyle's relationship to 17<sup>th</sup> century Cartesian mechanism. As has been previously mentioned, the Cartesian mechanistic conception of fundamental particles is the dominant account of matter in the 17<sup>th</sup> century, and it is the one embraced by those philosophers who wish to deny the autonomy of chemistry as a science and to advocate for the reducibility of its laws and explanations to those of physics. Such accounts of matter, including those found in textbooks, have little or no basis in experimental science and are usually theoretical and a priori since, according to the Cartesians, "deduction allow[s] finding general principles under which elements of knowledge [are] to be structured".<sup>49</sup> Although its theories have no experimental basis, Boyle believes that Cartesian mechanism provides the soundest alternative to the Peripatetic theory of substantial form and to the spagyric theory of the *tria prima* advanced by Paracelsus and other alchemists.

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<sup>47</sup> Clericuzio, "A redefinition of Boyle's chemistry and corpuscular philosophy", 577.

<sup>48</sup> Boyle, *Experimental History of Colours*, 152.

<sup>49</sup> Smets, "The controversy between Leibniz and Stahl on the theory of chemistry", 291.

In a number of key experiments, such as his work on the reintegration of potassium nitrate, Boyle deploys mechanistic corpuscularianism to explain how a heterogeneous substance can be analyzed into its component substances and how those components can be re-synthesized into the original compound. As he argues, if the theory of substantial form were correct, it would not be possible to reintegrate a heterogeneous substance like potassium nitrate once it had been analyzed into its constituent substances, because the substantial form would have been lost. Mechanistic corpuscularianism, on the other hand, entails the possibility of such reintegration because the fundamental corpuscles themselves are only endowed with the properties of shape, size, and motion. When substances are analyzed into their components and re-synthesized, the individual corpuscles retain their own individual mechanistic properties throughout each procedure. There is no loss of substantial form nor is there a transformation of mechanistic properties at the fundamental level, so the components into which a substance has been analyzed can unproblematically be brought together again to re-synthesize the original substance. Boyle also believes that a mechanistic and corpuscularian theory of matter can more successfully explain the process of transmutation and chemical transformation. In fact, for Boyle, mechanistic corpuscularianism actually entails the possibility of transmutation. Boyle argues this point at length in *The Sceptical Chymist*, a treatise primarily directed against the spagyrist's adherence to the theory of substantial form precisely because this theory does not offer an adequate explanation of why transmutation is possible. However, despite his allegiance to Cartesian mechanism, Boyle distances himself from the more extreme implications of this view. As has already been emphasized, Boyle accepts the ontological dependency of chemical properties on the mechanical properties of shape, size, and motion but does not endorse an epistemological and explanatory reduction of chemical properties to physical properties. Boyle's own commitment to the mechanistic particulate theory is, therefore, complicated by his desire to accommodate the notion of chemical properties into the context of his corpuscularianism. In order to do this, he has to develop a chemical ontology that allows for a theory of matter that is both mechanistic and non-reductionist. There are also suggestions, in Boyle writings, that he regards chemical properties not only as causally efficacious but possibly also as emergent properties that supervene on the mechanistic properties of fundamental material particles. Examples of this point are forthcoming in this essay.

In order both to endorse a Cartesian mechanistic theory of matter and to reject reductionism in favor of an emergentist theory of chemical

properties, Boyle's pragmatic solution consists of developing a hybrid theory of matter that distinguishes ontologically between fundamental corpuscles governed by mechanistic principles and non-fundamental corpuscular arrangements governed by chemical principles. His writings suggest that this complex theory allows him to (1) conceptualize more clearly the results obtained from his own chemical experiments, (2) assert the autonomy of chemical explanations from physical and mechanical explanations, and (3) assert the legitimacy of chemistry as an autonomous scientific practice independent from physics. Boyle's hybrid theory of matter distinguishes between corpuscles of the first order, which are endowed with strictly mechanical properties and are governed by physical laws, and corpuscles of the second and higher orders, which are endowed with causally efficacious chemical and generative (i.e., seminal) properties governed by chemical laws. It is interesting to note that this is very similar to the contemporary hierarchy between levels of description.

In *Of ye Atomick Philosophy* (1651-1653), Boyle explains his complex particulate theory by first equating atoms or fundamental corpuscles with *minima naturalia*, that is, with different particles that are not further divisible in nature. It should be clarified that his notion of *minima* differs from that of the Scholastics precisely because "Boyle rules out the Aristotelian notion of substantial form".<sup>50</sup> Rather, for Boyle, the properties of *minima* are to be understood as being strictly mechanical, that is, as being only the properties of shape, size, and motion. *Minima* are, therefore, the most fundamental particles of matter that obey strictly mechanistic physical laws. These particles can be called corpuscles of the first order because they are, ultimately, the particles upon which all phenomena depend ontologically. However, for Boyle, the questions inevitably arise of (1) how the properties of different chemical compounds can vary qualitatively and chemically, while the fundamental particles that constitute these compounds vary only quantitatively and mechanistically and (2) how one can explain mechanistically the causal efficacy of such chemical properties as acidity, alkalinity, salinity, and solubility, to name only a few. To answer these questions, Boyle ontologically expands his theory of matter by adopting the notion of non-fundamental corpuscular concretions that display chemical properties, what one can call corpuscles of the second order and of higher orders. We, thus, have an ontology of first-order corpuscles, or *minima naturalia*, which are the fundamental particles of universal matter endowed with the strictly mechanical properties of shape, size, and motion and of second (and higher) order

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<sup>50</sup> Clericuzio, *Elements, Principles and Corpuscles: A Study of Atomism and Chemistry in the Seventeenth Century*, 116.

corpuscles, that is, compounded corpuscles or corpuscular concretions endowed with chemical properties. Boyle explains this classification in his essay on *The Origin of Form and Qualities* by explaining that “there are also Multitudes of Corpuscles, which are made up of the Coalition of several of the former *Minima Naturalia*; and whose Bulk is so small, and their Adhæsion so close and strict, that each of these little Primitive Concretions or Clusters (if I may so call them) of Particles is singly below the discernment of Sense”.<sup>51</sup> According to Boyle, these primary concretions, or corpuscles of the second order, form clusters of an even higher order and “unlike *minima naturalia*, the corpuscles of the second order (and of higher orders) have not just mechanical properties, but chemical ones as well”.<sup>52</sup> In *The Sceptical Chymist*, Boyle uses the term “elementary corpuscles” to refer to *minima naturalia*, that is, corpuscles of the first order, and the term “compound corpuscles” to refer to corpuscular concretions, that is, corpuscles of the second and higher orders. In contemporary terms, corpuscles of the first order would be akin to atoms, while corpuscles of the second order would be akin to molecules. Just as Robert Mulliken claims that molecules have properties that their component atoms do not have, because he considers “a molecule to be a composite in which the atoms [loose] their singularity”<sup>53</sup>, Boyle believes that chemical reactions occur at the level of second and higher order corpuscles because these display chemical properties that are not displayed by corpuscles of the first order. Therefore, to the extent that first-order corpuscles are akin to atoms and that second-order corpuscles are akin to molecules, it seems that Boyle would be in agreement with Mulliken’s claims that “a molecule has properties which the atoms do not express and its decomposition gives again the separate atoms ... This molecular composite creates new homogeneous bodies starting from heterogeneous elements, which cannot be interpreted in terms of simple spatial vicinity of particles ... Thus the composite challenges the mere sum of the parts”.<sup>54</sup>

Boyle also believes that different concretions of primary particles with quantitatively different mechanical properties can express the same chemical properties, such as salinity for example. Boyle, in fact, “refrain[s] from establishing a direct relationship between a given quality

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<sup>51</sup> Boyle, *The Origin of Forms and Qualities*, 326.

<sup>52</sup> Clericuzio, *Elements, Principles and Corpuscles: A Study of Atomism and Chemistry in the Seventeenth Century*, 143.

<sup>53</sup> Llored, “Mereology and quantum chemistry: The approximation of molecular orbital”, 204.

<sup>54</sup> Ibid.



and a set of mechanical properties of the simplest corpuscles".<sup>55</sup> He, therefore, seems to regard the relationship between mechanical properties and chemical properties as an asymmetric dependence and to suggest that chemical properties of second and higher order corpuscles are supervenient upon mechanical properties of first order corpuscles or *minima naturalia*. "The supervenience argument would entail that if two compounds share the same macroscopic property ... we could not necessarily infer that the microscopic components from which the compounds are formed would be identical".<sup>56</sup> Although Boyle clearly affirms the ontological dependence of chemical properties on mechanical properties, "his aim [is] to reject the notion that sensible qualities [are] reducible to this or that ingredient of a mixed body. He present[s] the idea that a quality [has] relative character, namely, that it [is] generated from the constant interaction of different corpuscles, which themselves might not bear the quality in question ... Boyle also maintains that chemical qualities depend on the way in which the corpuscles that compose a body are disposed to act ... [and] denies that they directly originate from the mechanical properties of their primary particles".<sup>57</sup>

Boyle's many remarks regarding the producibility of chemical properties in compounds from ingredients that do not express the properties in question suggests that he endorses a notion of chemical qualities as emergent properties, ontologically dependent upon but not reducible to the shape, size, and motion of fundamental particles. For Boyle, the diversity in chemical and other sensible, macroscopic qualities arises or emerges from the specific manner in which first order corpuscles coalesce to form primary concretions or second order corpuscles. As Boyle explains, in *The Origin and Forms of Qualities*, it is from the structural disposition or "texture" of corpuscles

that the Colour, Odour, Tast, and other qualities of that Body are to be deriv'd, ... [from] the *Convention* and *Dissolution*, and the *Alterations* of them, from the *transposition* of their (suppos'd) Atoms ... And since, according to us, the various *manner* of the *Coalition* of several *Corpuscles* into one visible *Body* is enough to give them a peculiar Texture, and thereby fitt them to exhibit divers sensible Qualities, and to become a Body, sometimes of one Denomination, and sometimes of another.<sup>58</sup>

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<sup>55</sup> Clericuzio, *Elements, Principles and Corpuscles: A Study of Atomism and Chemistry in the Seventeenth Century*, 117.

<sup>56</sup> Scerri and McIntyre, "The case for the philosophy of chemistry", 225.

<sup>57</sup> Clericuzio, "A redefinition of Boyle's chemistry and corpuscular philosophy", 563-88.

<sup>58</sup> Boyle, *The Origin and Forms of Qualities*, 328-331.

It is likely that Boyle would agree with Newman's recent claim that "the generation of supervenient properties from subvenient ones that is so characteristic of the subject of chemical studies arises as a result of an interaction of parts that arises when such parts are in a certain configuration".<sup>59</sup> In fact, Boyle seems to have anticipated contemporary explanations for the supervenience of chemical properties on subvenient physical properties. In *The Mechanical Origine and Production of Volatility*, Boyle claims that "the same material parts of a portion of corporeal substance, which, when they were associated and contexted (whether by an *Archeus*, seed, form, or what else you please,) after such a determinate manner, constituted a solid and fixt body, as a Flint or a lump of Gold; by having their Texture dissolved, and (perhaps after being subtilized) by being freed from their former implications or firm cohesions, may become the parts of a fluid body totally Volatile".<sup>60</sup> Elsewhere, he states that "what ever be the number or qualities of the Chymical Principles, if they be really existent in Nature, it may very possibly be shewn, that they may be made up of insensible Corpuscles of the determinate bulks and shapes; and by the various Coalitions and Contextures of such Corpuscles, *not onely* three or five, *but* many more material Ingredients, may be compos'd or made to result ... that the very Qualities of this or that Ingredient flow from its peculiar Texture [or structural disposition]".<sup>61</sup> In his essay on *The Producibleness of Chymical Principles*, Boyle examines the various chemical properties of salts. When examining the specific property of solubility, Boyle claims that "a Disposition to be dissoluble in this or that liquor may be acquir'd by mixture and the new Texture of parts".<sup>62</sup> He then proceeds to give the examples of powdered sulphur and salt of tartar that, he claims, will not dissolve in spirit of wine (ethanol). He notes, however, that "if this Salt and Sulphur be mixt together, spirit of Wine will in less than an hour and sometimes in less than a quarter of that time dissolve enough of this matter to be richly colour'd by it, and this without the help of external heat".<sup>63</sup> He concludes from this experiment that the solubility of this mixture in spirit of wine, which is not a property of the component parts, is a property that

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<sup>59</sup> Newman, "Chemical supervenience", 54.

<sup>60</sup> Boyle, *Experiments and Notes About the Mechanical Origine and Production of Volatility*, 432.

<sup>61</sup> Boyle, *About the Excellency and Grounds of the Corpuscular or Mechanical Philosophy*, 112-4.

<sup>62</sup> Boyle, *Experiments and Notes About the Producibleness of Chymical Principles*, 34.

<sup>63</sup> *Ibid.*

*emerges from* the compounding of powdered sulphur and salt of tartar. Regarding the property of salinity, he reaches similar conclusions and claims that "whether we allow the *Epicurean* Hypothesis or the *Cartesian*; the first Saline Concretions that were produc'd by Nature must be confess'd to have been made of Atomes, or of Particles, that before their conjunction, were not Saline ... we may safely conclude, that salt may be made of matter, that was not salt before, and consequently that salt may be *de novo* produced".<sup>64</sup> Boyle here concurs with both Paracelsus and van Helmont that salts are producible from ingredients that are not salts but also implies that the property of salinity emerges from the particular structural disposition, or "texture", of the concretions and their interactions, and that this chemical property cannot be simply accounted for mechanistically and, in drawing a link between reliability and structure, Boyle clearly anticipates much of the current debate in philosophy of chemistry. The rest of Boyle's essay discusses specific experiments for the production of acid, volatile, and alkaline (or lixivate) salts. Boyle's famous experiment with the reintegration of potassium nitrate, while used to provide support for the mechanistic corpuscular theory of matter, is also used by Boyle to illustrate that the structural disposition or texture of concretions accounts for the chemical properties of a body and that, when these textures are altered by compounding the body with a differently textured body, the interaction of the different corpuscular coalitions will produce different chemical qualities.

To the extent, therefore, that the same fundamental corpuscles can, in principle, be compounded into differently structured higher order concretions whose chemical properties will vary according to the particular texture of that concretion, it follows that the chemical properties of a body cannot be simply deduced from or reduced to the mechanical properties of the individual first order corpuscles. Boyle's position aligns with the contemporary understanding of emergent properties as defined, for example, in the work of Shalizi and Crutchfield who establish that a property is emergent "if it is in some way novel or unpredictable, given the behaviours or properties displayed by the system's elementary components".<sup>65</sup> To the extent that, for Boyle, chemical properties clearly supervene on mechanical properties, this would suggest that for him chemical explanations are irreducible to physical explanations and that chemistry as a science is irreducible to and autonomous from physics. Boyle makes this plainly clear when he claims that "we can little better

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<sup>64</sup> *Ibid.*, 33-5.

<sup>65</sup> Newth and Finnigan, "Emergence and self-organization in chemistry and biology", 842.

give an account of the *Phaenomena* of many Bodies, by knowing what Ingredients compose them, than we can explain the Operations of a Watch, by knowing of how many and of what Metalls the Balance, the Wheels, the Chain, and other parts, are made".<sup>66</sup> The choice of this particular metaphor, that is, of a mechanism whose functioning cannot be accounted for simply by knowing its individual components, suggests that Boyle is probably responding to the unrelenting and a prioristic reductionism of Cartesian mechanists like Spinoza by emphasizing the point that *a facile reductionism is not entailed by an adherence to the mechanical philosophy*. For Boyle, dissolution, reintegration, volatility, fixedness, acidity, alkalinity, and other chemical processes and phenomena experienced in experimental work cannot be explained by simply relying on the fundamental physical properties of primary particles. He clearly believes that a mechanical understanding of *minima naturalia* is perfectly compatible with a complex theory of matter that allows for chemical explanations for those properties that are expressed in chemical reactions. He vigorously defends this compatibility by stating that "the mechanical principles are so universal, and therefore applicable to so many things, they are rather fitted to include, than necessitated to exclude, any other hypothesis, that is founded in nature, as far as it is so".<sup>67</sup> Since Boyle understands that the autonomy of chemistry as a science depends upon its epistemic irreducibility, he works to develop chemical, rather than strictly mechanical, explanations and he grounds these explanations upon a hybrid corpuscularian theory in which both mechanical and chemical properties exist and have causal efficacy.

## Conclusion

As established in this essay, Boyle anticipates many of the fundamental questions to be raised much later by philosophers of chemistry, questions of ontological and epistemological reduction, emergence and supervenience, and disciplinary autonomy but also questions regarding structural disposition, the relationality of properties, and the mereology of higher and lower levels of organization. As Harré and Llored have told us, "[s]ince Robert Boyle's corpuscularian philosophy, chemistry has been a mereological science. Displacing the metaphysics of 'continuous substances' and 'qualities' as the expression of 'principles', chemistry has

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<sup>66</sup> Boyle, *About the Excellency and Grounds of the Corpuscular or Mechanical Philosophy*, 111.

<sup>67</sup> Ibid.

been built on a 'part-whole' metaphysics."<sup>68</sup> The question that is being explored by some contemporary philosophers of chemistry is that of what sort of mereology, i.e., standard or non-standard, is applicable to chemistry, with the weight of philosophical support on the side of a non-standard mereology. Although Boyle himself is not involved in this sort of philosophical investigation, it is very likely that he would also side with non-standard mereology due to the fact that he does not fully embrace Cartesian reductionism. Had Boyle adopted a strictly *a priori* Cartesian interpretation of corpuscularianism and ignored the empirical findings of his own experimental work, he would have fallen prey to the reductionistic potential of a standard mereology, so that the "whole" must display only those properties that are inherent in its "parts" and any properties displayed by this "whole" must be entirely reducible to the properties of its "parts". As an experimental scientist, however, Boyle resists this approach. His own experimental work guides him in the direction of what we would call today a non-standard mereology. Boyle's experiment with the reintegration of potassium nitrate is particularly illustrative of this point, as are Boyle's writings on salinity in which he recognizes that "the first Saline Concretions that were produc'd by Nature must be confess'd to have been made of Atomes, or of Particles, that before their conjunction, were not Saline ... salt may be made of matter, that was not salt before, and consequently that salt may be *de novo* produced".<sup>69</sup> Boyle understands that properties of the "whole" are not always deducible from the properties of its "parts". Although, as a 16<sup>th</sup> century chemist, he lacks the proper philosophical vocabulary to articulate these ideas in mereological terms, some of his writing clearly anticipate some of the concerns of contemporary mereology as it relates to the philosophy of chemistry.

In his experimental writings, Boyle not only raises fundamental questions about dispositions, relational properties, and mereological relationships but also develops a hybrid ontology of first-order and second-order corpuscles to account for the experimental fact that higher levels of organization display properties that are not displayed at the lower levels. The purpose of this hybrid ontology, which embraces both a mechanistic conception of the lower ontological level and a non-reductionistic conception of the higher ontological level, is to explain the chemical phenomena he encounters in experimental work in a manner that is anti-reductionist and that accommodates the notions of emergence and supervenience of chemical properties. This hybrid ontology also allows

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<sup>68</sup> Harré and Llored, "Mereologies as the grammars of chemical discourses", 1.

<sup>69</sup> Boyle, *Experiments and Notes About the Producibleness of Chymical Principles*, 33-5.

him to defend the autonomy of chemical laws and of chemistry as an independent science, against the Cartesian view that dominated much of the 16<sup>th</sup> century debate on these issues. Although chemistry and chemical ontology have advanced far since Boyle's time, his views on the fundamental philosophical issues of reductionism, emergence, and the autonomy of chemistry seem very much in tune with the positions taken by many of the leading contemporary philosophers of chemistry.

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# DIDEROT, PHILOSOPHER OF CHEMISTRY, FROM THE ENLIGHTENMENT TO CONTEMPORARY SCIENCE<sup>1</sup>

FRANÇOIS PÉPIN

## 1. Epistemology and the Role of History in the Philosophy of Chemistry

That the epistemology and philosophy of science gains from placing itself in an historical context is the point of view widely held in the French academic tradition. This historical epistemology may be seen in Meyerson's work on chemistry. Yet the philosophy of science has become a specialised domain, wherein the historical perspective is at times voluntarily greatly limited. It is thus that the "philosophy of biology" is often separated from its historical context to focus on contemporary scientific research. What orientation might one take for the philosophy of chemistry? Should it be a philosophy working from the base of an historical epistemology, including precise historical accounts, or a philosophy oriented exclusively towards the world of contemporary scientific research? In the open, collegiate spirit of this volume, indeed emulating that spirit of the Lumières françaises, I will seek to demonstrate the relevance of Diderot's experimental philosophy to consider chemistry, from the starting hypothesis that this might enlighten our understanding of even the most contemporary research in the field.

But this brings up a particular paradox: Diderot studied chemistry prior to the "scientific revolution" of Lavoisier. Diderot took a passionate interest in the chemistry of his day, the *arts chimiques* or the chemistry of the *arts et métiers* such as metallurgy and dyeing. Diderot followed Rouelle's celebrated demonstrations in the *Jardin du Roi*, now the *Jardin des plantes* in Paris. But although Lavoisier also attended these important lectures, it remains—from an historical and epistemological point of view—that Diderot contemplated "pre-lavoisian" chemistry. Lavoisier's

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<sup>1</sup> Translated by Christopher Jarvis with the author.

concept of a chemical element, or *corps simple*, and his insistence on systemic measurements are often opposed to the qualitative dimensions of his predecessors. This, however, merits a more nuanced approach. As recent studies of chemistry during the period of the Enlightenment have shown, indeed dating back to Meyerson<sup>2</sup> in the early 20<sup>th</sup> century, chemistry did not await Lavoisier to undertake quantitative measurements, to point out the difficulties with the concept of the element and *mixtes*, or mixtures, nor to reflect upon the interface between chemistry and other physical and natural sciences. Nonetheless, there is a completely novel scientific configuration regarding chemistry today. This begs the question as to what relevance might Diderot's philosophy have upon the advances in chemistry that followed. The difficulty is further magnified when we envisage chemistry throughout the course of its history, wherein the very definition of what entails chemistry has been in constant flux.

A philosophical point of view should, however, allow for the establishment of relationships within a field during its flight through history. If the concept of the philosophy of chemistry is to hold any meaning, the exploration of such issues cannot be halted by the course of events. As such, the philosophy of physics may draw from the diverse works of Galileo, Descartes or Newton. But this is not only a question of historical record. Observation of the works from different periods in their historical setting elucidates the *philosophical decisions* taken that construct the debates and directions of continued scientific inquiry. Moreover, a large historical point of view is the ideal remedy for the return of the essentialisation of issues in a *philosophia perennis* of sciences.

It is thus interesting to envisage an historical epistemology as a starting point for the philosophy of chemistry. In adopting this approach to examine the philosophy of Diderot, we are following his precedent. Indeed, Diderot integrated an historical dimension to an epistemology and a philosophy greatly influenced by chemistry. Having followed Rouelle's courses for three years, Diderot composed extensive notes. Inspired by the article "Chymie" written by Venel for the *Encyclopaedia*, Diderot wrote an introduction putting the courses into an historical perspective. Therein, he stressed what I have called the *scientificité* and the *dignité philosophique* of chemistry. I will therefore seek in this article to reveal Diderot as a philosopher of chemistry and as an historical epistemologist

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<sup>2</sup> *Identité et réalité*. (1908, 1951). Paris: Vrin and *De l'Explication dans les sciences*. (1921, 1995). Paris: Fayard.

who followed in the footsteps of Fontenelle<sup>3</sup>. The originality of Diderot springs forth from his chemical point of view that led his attention to the diversification of different fields of science and the tensions between them. It is thus an historical epistemology multiplying the different exercises of scientific research that animates his philosophical approach to chemistry.

In revisiting Diderot's work on chemistry in its historical context more is revealed than the philosophy of the Enlightenment. Without proclaiming Diderot to be a precursor, an examination of how certain difficulties in chemistry and its philosophy were dealt with during his time echoes true today and provides a valuable precedent for better framing interrogations of current issues in the field. Diderot never approached chemistry with preconceived notions, nor did he attempt to use discoveries in the field to defend a philosophy formed elsewhere. Rather, Diderot found in chemistry a natural partner for his philosophy. Chemistry provided for him a novel philosophical starting point. The following discussion proposes, therefore, a reflection not upon the individual concepts and discoveries laid out by Diderot, but rather an examination of his view of chemistry and his use of chemistry as a starting point for philosophical debate.

## 2. The Ever-shifting Identity of Chemistry

Several analyses of Diderot demonstrate an original point of view on epistemology and philosophy, a point of view greatly influenced by his interest in chemistry. Rather than simply taking the results of his contemporaries' research, Diderot formed his ideas from the point of view of a chemist. Starting with the manner in which Diderot saw the unique nature of experimentation in chemistry, where he characterised chemistry as a terrain science, a field science or an earth science. But what defines the terrain of chemical research? How does its nature as an experimental field relate to its philosophy?

### 2.1. Chemical Terrain

Where does chemistry take place? By the Enlightenment chemists had well established their field as an experimental science whose progress sprang forth from the laboratory. In contrast to theoretical physics and

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<sup>3</sup> In the *Histoire de l'Académie Royal des Sciences de Paris*. Fontenelle wrote reviews of the scientific "mémoires", prefaces and eulogies of the dead scientists as "Secrétaire perpétuel" of the Academy from 1699 to 1740.

systematic philosophies, research in chemistry was conducted in direct contact with nature<sup>4</sup>. But as Diderot points out, the domain of chemistry is not limited to the laboratory. Rather, it is encompassed in a practical methodology of inquiry. Thus a chemical point of view can be framed in almost every field, the chemical terrain being infinitely extended and reconstructed. But it does not imply any reductionist epistemology. For instance, Diderot proposes analogies that go beyond the transpositions of the alchemists and iatrochemists. In comparing organic matter with chemical reactions from the laboratory Diderot is not seeking to reduce life to chemistry, but rather to observe organic matter through the eyes of a chemist and to take the matter quite literally in hand.

In *Pensées sur l'interprétation de la nature*, Diderot is inspired by the chemistry of *arts et métiers* to valorise manual labour as a means for gaining knowledge. Working from practical experience, the fruits born by the chemist's labour demonstrate the validity of "tâtonnement"<sup>5</sup> or touch. Indeed, Diderot proposes a sensory epistemology that seeks to reform the tactile. Diderot opposes the methodology of the chemist with that of more theoretical fields, where dependence upon a Cartesian, geometric model requires a complete visualisation (at least through imagination) for comprehension. In working directly with his hands, the chemist is able to continue in his research and circumvent the insurmountable variety and constant flux presented by nature; the chemist can continue his work without seeing everything and can even at times execute experiments blindly<sup>6</sup>. In his rehabilitation of touch, our hands as a sense organ, Diderot does not intend to abandon sight as a sense in service to the actions and observations of the scientist. Rather, it is seen as the vision of the practised eye of an expert surveying his experiment, or in a broader sense nature itself.

In a later text, Diderot expresses these elements by opposing the universal laboratory revealed by chemistry and direct experience with the mere abstractions created by those whose models are based solely upon their thinking:

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<sup>4</sup> The opposition between the *cabinet* (the study) and the *laboratoire* is a leitmotiv of philosophers of chemistry and chemists following the tradition of Becher and Stahl. See for instance, Rousseau, *Institutions chimiques* (1747?), I, 1.

<sup>5</sup> Word often used by Diderot, which could be translated by trial and errors or tentative research.

<sup>6</sup> See in particular *Pensées sur l'interprétation de la nature*, 1753-1754, XXI-XXXI. See also the *Lettre sur les aveugles* (1749).

Undertake geometry<sup>7</sup> and metaphysics as you please, for myself, as a physician and chemist, who addresses matter in nature and not in my imagination, I observe matter in its diverse forms and actions, behaving in the universe as in the laboratory, where a spark might hardly find itself next to three molecules of saltpeter, carbon and sulphur without resulting in a necessary explosion<sup>8</sup>.

From Diderot's early interest in the chemistry of the *arts mécaniques* sprang forth his conception of the laboratory. In this conception, any location where a controlled transformation of matter might be undertaken is the chemist's terrain. Staking claim to territory outside of the laboratory immediately provides a response to challenges that discoveries made in an artificial setting might not apply in nature at large. This question, confronted since the beginning of experimental physics, is of central importance to chemistry, which produces its *objects* and not only its phenomena. "Fire creatures" provide a typical example from the classical period: does the fire of chemical distillations or decompositions merely reveal the components that were already present in a material by breaking them down, or does it create novel entities from that of the originally examined material<sup>9</sup>? As demonstrated by numerous articles in the *Encyclopaedia*, Diderot perceived these technical processes as fresh terrain for chemistry, permitting it to break free from the confines of the laboratory. Though historical distinctions must be made, this dimension of chemical practice is remarkable for its continuity from 18<sup>th</sup> century artisanal work to industrial chemistry of the 19<sup>th</sup> century, perhaps even continuing today in the modern chemistry of *Big Science*. Chemistry takes place in a variety of settings, blurring the distinctions between what is artificial and what is natural. In the practice of chemistry, artifice and nature are not parallel settings as in the mechanics of Descartes, but rather intertwined. Thus the division between pure and applied science—though it

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<sup>7</sup> "Geometry" means here physico-mathematical sciences that consider nature from abstract principles. More particularly, Diderot aims at Cartesian mechanics that reduces matter to extension and separates it from movement. This criticism does not imply that Diderot refuses any relevance of mathematics in natural sciences.

<sup>8</sup> *Principes philosophiques sur la matière et le mouvement*, rédigés en 1770, *Œuvres philosophiques*, Classiques Garnier, p. 395. "Vous ferez de la géométrie et de la métaphysique tant qu'il vous plaira; mais moi, qui suis physicien et chimiste; qui prend les corps dans la nature, et non dans ma tête; je les vois existants, divers, revêtus de propriétés et d'actions, et s'agitant dans l'univers comme dans le laboratoire, où une étincelle ne se trouve point à côté de trois molécules combinées de salpêtre, de charbon et de soufre, sans qu'il s'ensuive une explosion nécessaire."

<sup>9</sup> Boyle's *Sceptical Chymist* stressed this issue in 1661, but it is an old question.

had been proposed by an 18<sup>th</sup> century chemist<sup>10</sup>—softens, particularly for Diderot who stressed the valour of chemistry’s experimental approach.

This leads to a new concept of chemistry’s domain. Rather than concentrating on the organisation of a single defined work area, Diderot aims to study chemistry through its productions and its regular expansion into new terrain. Diderot was not driven simply by his historical setting; besides, although the modern laboratory has certainly become more sophisticated, Enlightenment laboratories already consisted of an assortment of specialised equipment.<sup>11</sup> For Diderot, the chemist’s place is in his active experimentation in direct contact with matter. His writings abound in images of practical laboratory work: “crumbling manipulations” when “blindly ploughing” into the “subterranean.”<sup>12</sup> An article from the *Encyclopaedia*, “Subterranean Geometry,” extends the roots of these practical techniques further with regards to mineralogy and mining: there is a specific geometry to the organisation of evolving, expanding space of the mine. Likewise, the chemist workspace is not defined in advance; it is constantly constructed, expanded and reconstructed. The subterranean image holds a particular power here, in a classic dichotomy proposed by some chemists as early as Becher: in physics the surfaces of bodies are designated properties limited to their shape or geometric form without entering into their subterranean depths<sup>13</sup>, whereas the chemist looks beneath the surface.

It is this image of the terrain of chemistry, rich in its depth that defines chemistry amongst the sciences. Contradicting the position taken by d’Alembert in the *Encyclopaedia*, Diderot refuses to envisage chemistry as a subaltern in a hierarchical scheme of the sciences<sup>14</sup>. Rather, Diderot sees

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<sup>10</sup> See Bernadette Bensaude-Vincent. (2008). *Matière à penser. Essais d’histoire et de philosophie de la chimie*. Paris: Presses Universitaire de Paris Ouest, p. 175-183.

<sup>11</sup> A good illustration is the *planche* representing the chemical laboratory in the *Encyclopaedia*.

<sup>12</sup> *Pensées sur l’interprétation de la nature*, XXI.

<sup>13</sup> This opposition is recurrent in the writings of Rouelle’s students like Rousseau, Diderot and Venel. It was first formulated by Becher, who is quoted by Diderot in the *Plan d’une université* (written for Catherine II, Empress of Russia): “Le chimiste Becker a dit que les physiciens n’étaient que des animaux stupides qui léchaient la surface des corps, et ce dédain n’est pas tout à fait mal fondé.” (*Œuvres complètes*, Assézat et Tourneux (éd.), 1875-1877, III, p. 463). (“The chemist Becher said that physicists were stupid animals licking the surface of bodies, and this disdain is not totally unfounded.”)

<sup>14</sup> See *Corpus, revue de philosophie*, n° 56, 2009, “La chimie et l’*Encyclopédie*”, C. Lehman et F. Pépin (ed.), especially the introduction by the editors.

chemistry as a field that is constantly shifting, regularly drawing from other sciences through new and evolving relations. It is thus that any tentative to create a hierarchy of sciences is undermined. Furthermore no topic can be exclusively allocated to one science or means of inquiry: there is no definitive sharing out of territories. It is perhaps here that Diderot best demonstrates his historical sense of the evolution of science. In this defence of chemistry as a specific, experimental and practical science, its relations with other sciences and its historical context are not in any way abandoned. The lively roadmap of sciences proposed by Diderot may be opposed with the ascending ladder of scientific fields defined in a strict hierarchy of level and nobility. Diderot stresses the *depth* of chemistry, without in anyway seeking to degrade its status. Chemistry is also a subtle science, notably in studying organic matter, a science of “airs” or gases and of colour. Chemistry runs the gamut from microscopic to macroscopic, employing techniques from many different sciences and arts. Chemistry is at the crossroads of many scientific terrains.

## 2.2. Reduction and Irreducibility

In inviting us to reconsider how different scientific fields interact, Diderot provides a starting point that is particularly pertinent for the philosophy of chemistry, both historical and contemporary. Underlining the practical and experimental specificity of chemistry, Diderot keeps a certain distance from the question of the reduction between theories. Today, we often ask if all of chemistry might be reduced to quantum mechanics, thus becoming completely engulfed by physics. Already during the period of the Enlightenment a “rational mechanics” employing the tools of Newtonian physics and mathematics posed a similar challenge to all other scientific endeavours; Diderot addressed this challenge. But in his philosophy of chemistry, rather than contesting the theories of physics and their implications upon chemistry, Diderot considers chemistry through its own unique form of labour. It is in starting from the *practice* of chemistry that grows forth the scientific inquiry specific to the field, not in accepting the questions of physics and the philosophy of physics. The question of the irreducibility of chemistry may thus be seen from two different viewpoints. On the one hand, there is the issue of the reduction of the laws and concepts of chemistry to the ones of a more fundamental science. On the other hand, the irreducibility of chemistry may be defined as a manner in which to pose questions constructed around a *savoir-faire* specific to the instruments and tools of the chemist’s laboratory.

Concerning the reduction of chemical affinities to gravity, Diderot maintains the argument promoted by chemists such as Venel in refuting the application of the law though some changes in the parameters (for the tiny distances involved in chemical interactions, the cube of the distance instead of their square<sup>15</sup>). He sides with Venel as it would imply accepting the premises of the physico-mathematical reduction. Attempting to bring chemical affinities into line with the law of gravity ignores the fundamental problems faced by the working chemist in the laboratory. In addressing the concept of chemical affinities, the chemist must conceive of a multitude of attractions taking place in mixtures-chemical combinations of substances, each substance in the mixture carries with it its own particularities and its own interactions with its neighbours. Venel and Diderot consider that chemical affinities might be explained by some form of attraction, but it requires a plural and specific view of the concept going beyond a simple application of the universal law of gravity.

In transposing Diderot's argument onto more contemporary science, the philosophy of chemistry must ask what practical applications quantum mechanics might have in the laboratory. Or more generally, what relationship should chemistry maintain between its own practical operation and any new discoveries that may prove to be instrumental for new operations, productions or theoretical understanding? Stretching this argument to an extreme, it is possible to affirm that the question of the reducibility of chemical equations and reactions to quantum mechanics is the terrain of the physicist, not the chemist. It is for the chemist to query the utility of quantum mechanics in as much as how it may be put to service in the practice of chemistry. Thus the status of chemical concepts is determined by the role they play in the practice of chemistry rather than a grand inter-theoretical reductionism such as has been proposed since the Vienna Circle<sup>16</sup>. Eric Scerri has stated that those authors that dedramatize the problem of the reduction of chemistry to physics were themselves historians<sup>17</sup>. But there is a philosophical viewpoint of this question,

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<sup>15</sup> Newton suggested this question, but, above all, it stems from posterior mechanical writings concerning astronomical issues and the reduction of any kind of apparent attraction to gravitation, including affinities. In France, Buffon criticized in 1745 Clairaut's hypothesis of a variation of the exponent of the law, and proposed in 1765 to universalize this unique gravitational law to chemical affinities, with the intervention of new factors such as the form of particles.

<sup>16</sup> Logical positivism has defended the principle that in the final analysis any knowledge comes from experience. But, regarding this question, it handed down above all a logical program trying to derivate the statements of a science from those of a more fundamental science.

<sup>17</sup> "The Ambiguity of Reduction", *Hyle*, vol. 13, n° 2, 2007, p. 68.



buttressed by history without being exclusively dependent upon it, that highlights the specificity of a line of inquiry fuelled by the practice of chemistry of itself. This, in any case, is the legacy offered to us by Diderot.

This philosophical approach converges with the intuitions of chemists such as Venel on the *irreducibility* of chemistry due to its own practice bringing forth its unique type of theoretical effort. It is the specificity of the chemist's work that permits the philosophical perspective laid out by Diderot to overcome the challenge of *de facto* reductionism to a particular physical basis whilst affirming the irreducibility of chemistry due to its practical specificity. It is therefore possible to find some extension of this attitude when philosophers of chemistry propose a certain irrelevance of the determinations of quantum mechanics in order to deal with what interests the chemist: the relationships between substances in an experimental culture. But I would like to stress the value of a refusal of the universalization of physic's issues, be that rational mechanics during the Enlightenment or quantum mechanics today. This stance circumvents being trapped in a position doomed to be overrun by the course of historical developments in the sciences whilst contenting itself to point out the inadequacy of the produced reduction.

The same sort of distinction may be used to address the question of emergence. Taking a common approach, in terms of the emergence of new properties from the increasing complexity of a system of entities, a series of levels from *micro* to *macro* assume a hierarchy ranging from the fundamental building blocks of the *micro* scale up to the macroscopic. The question is then to know if the *micro* determinates the *macro*<sup>18</sup>. This view of the issue asks if the sum of the parts and their relations can explain the whole, emergence being the apparition of novel properties on the systemic level that were completely absent on the level of individual elements. Diderot asks instead how the *micro* and *macro* might interact and whether elements might already possess the potential for different properties that are only revealed in the context of certain complex systems. In particular, Diderot's interest in *vitalist* medicine provides an interesting response. Diderot does not refer to any "transcendent" or vital force in living matter, rather, he seeks to understand the specificity of the living *milieu* and the entanglement of the levels of organisation: molecule; fibre; organ;

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<sup>18</sup> This is what Mario Bunge names the micro-reduction (*Emergence and convergence. Qualitative Novelty and the Unity of knowledge*, University of Toronto Press, 2003). M. Bunge puts forwards the limits of this kind of reduction, and underlines the paradox that it often relies on quantum mechanics thought the standard interpretation of quantum mechanics is rather macro-reductionist.

organism<sup>19</sup>. Whilst avoiding the creation of a *biological exception* for chemical operations, Diderot nonetheless seeks to interrogate the novel potentials of elements revealed when found in living matter. Thus, rather than seeking to reduce biology to a series of chemical processes, Diderot asks what happens to chemical materials when placed in a living matter, or a “vital” context. Rather than building up from the *micro* level of elements, Diderot seeks the effects of this specific organic environment upon chemical transformations, and how these might be affected by alternate states: sickness/health, genesis/growth/ageing, etc. Diderot insists upon the cyclical nature of living matter, often beyond the capacities of 18<sup>th</sup> Century scientific knowledge<sup>20</sup>, addressing chemical transformations such as digestion and fermentation<sup>21</sup>.

Altogether these lead back to the question of the identity of chemistry. Diderot’s lines of inquiry liberate chemistry from the need for its own unique object of study. If the identity of chemistry lies at the very heart of the historical development of the field<sup>22</sup>, this is because it is in constant flux. But is there a basis upon which chemistry can stabilise itself in response to this ever recurring identity crisis? Diderot conducts us towards an image of chemistry constantly adopting new techniques and pushing at the frontiers of neighbouring fields of sciences. His definition of chemistry replaces the need to define its object of study with its constant fabrication of novel objects. This fabrication of novel objects is a product of the laboratory culture of the chemist, a point of great importance to Diderot. The oral and tacit history of this experimental culture is extremely fragile, yet being literally handed on in a *tactile* sense during demonstrations and during the execution of work in the laboratory it is essential to the

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<sup>19</sup> See in particular the *Rêve de d’Alembert*, written in 1769, which relies on chemistry and medicine, especially physicians from the school of Montpellier like Bordeu and Menuret de Chambaud. See F. Pépin. (2011). “Vitalisme, chimie et philosophie autour de l’*Encyclopédie* et Diderot”, in P. Nouvel (ed.), *Repenser le vitalisme. Histoire et philosophie du vitalisme*. Paris: PUF, p. 131-143.

<sup>20</sup> See in the *Rêve de d’Alembert*, the example of the marble reduced to powder becoming humus, vegetal, animal then probably dust again. This example is exaggerated on purpose and is followed by more precise analysis of the processes of transformation.

<sup>21</sup> About the chemical way to practice “horizontal” explanation in distinction with “vertical” explanation, see Roald Hoffmann. (2007). “What might philosophy of science look like if chemists built it?”, *Synthese*, vol. 155 (3), p. 321-336, paragraph 5. The way R. Hoffmann’s underlines the circulation of explanations and the crossing between different fields reminds of Diderot.

<sup>22</sup> See the history of chemistry by Bernadette Bensauode-Vincent and Isabelle Stengers. (1993). *Histoire de la chimie*. Paris: La Découverte.

definition of chemistry. Today, when defining the terrain of chemistry presents a greater challenge than ever, when neither its subjects of study nor its techniques are unique to the field, the most enlightening point of view may be to look towards the actual practice of chemistry and the fields where this practice is called upon. With Diderot, we might look at the *chemistry* of things. In this sense, *chemistry* is the dimensions or characteristics of an object, best revealed and worked with by the methodology handed down in the laboratory culture of the chemist.

### 3. An Ontology of the Qualitative

At present, the question of phenomenal or ontological specificity seems to have abandoned chemistry in order to concentrate upon the study of biology. It might even be seen as an inversion of the position of chemistry, in particular since the “physico-chemical” determinations discussed by Bichat, which has been seen to become a reductionist science, or citing Canguilhem<sup>23</sup>, “imperialist”. However we may judge these assumptions, what role might remain for a philosophy of chemistry that highlights the qualitative dimensions of matter and chemical operations as proposed by Diderot?

Diderot’s interest in the qualitative element of chemistry is an element of 18<sup>th</sup> Century science that appears completely dated today. Without assuming the erroneous cliché that quantification only began in chemistry with Lavoisier and the affirmation of Bachelard that the chemistry of that time was a purely technical field devoid of scientific inquiry, addressing the qualitative element of this science poses a real difficulty. Doesn’t scientific rigour stand to gain from quantification? Isn’t the modernity of philosophy and science built upon the reduction of observation to primary qualities that may be expressed numerically and thus submitted to mathematical manipulation? Colour, for example, can be reduced to a correlation: an arbitrary ranking of intensity of absorption at a given wavelength of light as we understand it today, or a certain “surface porosity” as it was explained by Descartes. Chemistry throughout its own history has sought to abandon qualitative observation in favour of quantification. Since quantum chemistry has provided a new mathematically coherent model for chemical interactions at their most fundamental level, how, and furthermore, *why*, might we rescue the role qualitative observation in old chemistry?

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<sup>23</sup> Canguilhem, Georges. (1998). “Aspects du vitalisme”, in *La Connaissance de la vie*, second edition. Paris: Vrin, p. 95.

Nonetheless this is one of the historical and epistemological themes that brings forth the most contradictions, oversimplifications and miscomprehensions. The first merit of an epistemology such as Diderot's would therefore be to put things in a clearer perspective. But I would like here to go further: as formulated by Bernadette Bensaude-Vincent<sup>24</sup>, there exists a treatment of realism unique to chemistry. Associating the question of the scientific and philosophical treatment of qualities, Diderot reformulates the question of epistemological realism, i.e. do scientific concepts correspond to a reality, and of metaphysical realism, i.e. can our representations gain access to reality itself, and how might we even know if we had?

First, the flagrant error of Bachelard<sup>25</sup> that finds itself repeated insidiously elsewhere must be addressed. The vast majority of 18<sup>th</sup> Century chemistry, most certainly its core set of advances, does not consider the objects of perception as realities. Chemists of this period do not assume the existence of a real entity corresponding to every perception, be they direct sensory perceptions or those obtained through instruments. Although phlogiston might be responsible for colour, this lies in its interactions with other substances as phlogiston itself was thought to be colourless. This example illustrates the displacement of characteristics, in this case colour, from one substance in a mixture to another. If colours are treated as realities and not only perceptions, it is that colour may be transferred from one body to another in a mixture, it may intensify or weaken in function with its environment and what other substances are present therein<sup>26</sup>. Care must be taken in its manipulation, as in some cases the colour may be *burnt out*, for example in the manufacturing of painted porcelain. The qualitative aspects of this chemistry were *actions*, changes and operational causalities that do not come under those criticisms classically applied to the realisation of sensory perceptions. The chemist's passive observation of colour are not what anchors its reality, rather it is its active manipulation which shows what colours can do and what we can do with colours.

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<sup>24</sup> For instance in *Matière à penser*. See also Roald Hoffmann. (2007). What might philosophy of science look like if chemists built it?, *Synthese*, vol. 155, n° 3, p. 321-336, paragraph 4.

<sup>25</sup> In particular in *La Psychanalyse du feu*, Gallimard, 1949, reissue Folio Essais, 1989, chapter V: "La chimie du feu: histoire d'un faux problème" (The chemistry of fire: a history of a wrong issue).

<sup>26</sup> See the *Cours de Rouelle* written by Diderot, *Œuvres complètes*. Paris: Hermann, IX, p. 227.

That being stated, two different forms of qualities must be distinguished, as well as their subsequent influences upon the epistemology of chemistry. Qualitative sensory perception was often put forward as a defining characteristic, as a sign of real properties, for example chemists would taste salts to classify them. An ontological interpretation of that method requires a conception of reality as an encounter between objects and our senses, refuting the possibility that our senses might be confounded. This link between common sensory perception and scientific knowledge is supported in the works of both Diderot and Meyerson. But it is when qualities are *active* that chemistry comes into play. Chemistry is the study of interactions between substances, their changing relationships in mixtures for example. This leads to the idea that qualities are actions and that actions are qualities inherent in materials' interactions. Here, I would like to stress the epistemological power of this viewpoint, in particular its pertinence to the philosophy of chemistry. This puts in perspective the problem brought up by Joachim Schummer: is chemistry a study of substances or of reactions<sup>27</sup>? Diderot marries the epistemological debates with a philosophical attitude that reinvigorates the qualitative, breaking with the classic model of representation.

Bensaude-Vincent<sup>28</sup> demonstrated that the classical issue of epistemological realism owes itself to a physical conception. It fits more widely into the scheme of representation, with the opposition between, on the one hand, concepts and scientific theories conceived as representations of the subject and, on the other hand, nature considered as object. Far from being the mainstream of modernity, Diderot's reflections upon chemistry undermined this concept in the 18<sup>th</sup> Century. The same might be said for the division between primary and secondary qualities. Thus, there is an alternate modernity focused on chemical issues concerning qualities. This brings us to two questions. First, can chemistry do without the qualitative? And second, does chemistry undermine a certain concept of modernity in science and philosophy?

The most original point of view presented by Diderot, a conception that dismantles the division between primary and secondary qualities, consists of treating forces and movements as qualities of heterogeneous substances. These properties, when treated numerically in physics, become a *quality of a substance*, "Movement is not an action, it is a quality, a property, etc.: and the action is its effect<sup>29</sup>." This idea has far reaching

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<sup>27</sup> See for instance the editorial dealing with this issue in *Hyle*, vol. 10, n° 4.

<sup>28</sup> *Matière à penser*, p. 40-64.

<sup>29</sup> *Observations sur Hemsterhuis*, written in 1773-1774, *Œuvres de Diderot*. Paris: Laffont, t. I, p. 707.

implications. On one hand, it places itself in a materialist philosophy playing chemical determinations against certain physical determinations of a passive substance. On the other hand, this brings up an interesting difficulty faced by any epistemology and philosophy of chemistry: can the study of forces and the properties that manifest themselves during the course of chemical reactions stand without a material support, or more precisely, can it break free from a theory of substance? This poses the question of the materiality of operational qualities in chemistry. The alternative would be to stop at the operations and effects, or reactions, in making these the sole object of study in chemistry. This attitude resembles that of the physicist and mathematician d'Alembert, who reduced attraction to its effects in proposing a rational system of mechanics where the concept of force is ceded to a rapport between effects. But the philosophical gesture of Diderot would seem more appropriate to a philosophy of chemistry. Indeed, how could a chemist eschew the materiality of the qualities upon which he works? How could he not question the relationships between interacting *things*?

This leads to Diderot's concept of the element, which is not an analytical term, nor an irreducible body, but rather a substance defined by its qualities. Each material bears certain properties:

But in resting my eyes upon heaped bodies of matter; I see everything in action and reaction, destroying itself in one form to be recomposed in another, sublimations, dissolutions and combinations of every sort, phenomena incompatible with the homogeneity of matter. From which I conclude that it is heterogeneous, that nature contains an infinity of elements, each of these elements by its diversity has a particular force, innate, immutable, eternal, indestructible, and that these forces within each body take effect outside of themselves: from where the birth of movement, or rather a general fermentation in the universe<sup>30</sup>.

The nature of the element, its definition in relation to operations and theories, is integral to the history of chemistry as a science. But as

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<sup>30</sup> *Principes philosophiques sur la matière et le mouvement*, p. 398. "Mais j'arrête mes yeux sur l'amas général des corps ; je vois tout en action et en réaction ; tout se détruisant sous une forme ; tout se recomposant sous une autre ; des sublimations, des dissolutions, des combinaisons de toutes les espèces, phénomènes incompatibles avec l'homogénéité de la matière ; d'où je conclus qu'elle est hétérogène ; qu'il existe une infinité d'éléments divers dans la nature ; que chacun de ces éléments, par sa diversité, a sa force particulière, innée, immuable, éternelle, indestructible ; et que ces forces intimes au corps ont leurs actions hors du corps : d'où naît le mouvement ou plutôt la fermentation générale dans l'univers."

Meyerson to a certain measure proposes, Diderot posits that the chemist cannot divorce himself from the definition of materials by their intrinsic qualities. Thus Diderot stresses the particular importance of the potential contained within a given material. This potential is constantly revealed as the material is placed into different contexts and in relation with different materials. The most audacious example being the universal sensibility of matter<sup>31</sup>, but Diderot envisages this for affinities as well. There is no contradiction in this framework between the materiality of forces and their variation. Diderot stretches this to the utmost in his view of the constant flux in nature, “There are as many diverse laws as there are varieties of the force within each elementary molecule that constitutes a given body<sup>32</sup>.”

The ontology of the qualitative allows us to consider that chemistry not only has its own ontology, but also its own metaphysics: it elaborates a fresh treatment of metaphysics apart from the mainstream traditions of philosophy. Often overlooked in the history of ideas is the fact that the subversion of the Cartesian tradition, and more broadly that of classical metaphysics, by philosophers such as Diderot is buttressed by the study of chemistry while revealing its full philosophical potential.

#### 4. A Philosophy of Substance

Chemistry serves as a foundation upon which Diderot formulates a philosophy of matter. The way Diderot considers matters shows the originality of his materialism in comparison with the other materialisms of the Enlightenment and the following centuries. Against the classical metaphysics and the physics of his time, Diderot promotes a pluralisation of different classes of matter: matter is the only substance but it is plural. The problem we inherit from Diderot’s philosophy of chemistry consists of multiplying the different classes of matter when conceiving natural transformations whilst maintaining the substantiality of forces and qualities. This requires a separation with the metaphysical substance

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<sup>31</sup> In the *Rêve de d’Alembert*, Diderot proposes the hypothesis of sensibility as a universal property of matter. He distinguishes an actual sensibility present in living bodies and a potential sensibility present in any matter (or any material). Sensibility becomes a property distributed in various degrees corresponding to different contexts or different processes of actualization. The model is first physical (with the distinction between “force vive” or kinetic energy and “force morte” or potential energy). But it is above all chemical. Chemistry allows conceiving the crossings between kingdoms thanks to processes of transformation freeing latent properties such as sensibility.

<sup>32</sup> *Principes philosophiques sur la matière et le mouvement*, p. 396.

considered as an abstract homogeneous substratum, but also with the so-called disappearance of matter being superseded by energy or information.

Two modern questions may gain from being seen in this light. On the one hand, modern materialism has for the most part abandoned chemistry<sup>33</sup>. It tends to put matter aside, or treats it as a philosophical “category” that has been estranged from any scientific investigations. This may be seen in the materialism of evolutionists as well as in contemporary Marxist currents—Engel’s dialectic of nature been largely, and perhaps justifiably, abandoned today. Joachim Schummer evokes one notable exception<sup>34</sup>, the Soviet tradition descending from Engels of a non-reductionist perception of the plurality of sciences, an epistemology well adapted to chemistry. A “dialectical philosophy of chemistry” has thus stood as a guard against what Marxists saw as a French mechanistic materialism—which is very questionable, this materialism being sustained by chemistry as we can see in the works of Diderot and also d’Holbach, several anonymous manuscripts, etc. But this dialectic otherwise seems to be rather an application about chemistry of a philosophical schema deemed universal rather than a philosophical reflexion springing forth from an interest in chemistry.

On the other hand, the modern philosophy of chemistry seems to neglect the monolithic concept of matter as perhaps overly metaphysical. An alternative route would be to study particular materials, as demonstrated by Bensaude-Vincent<sup>35</sup>. But the concept of matter against which materials might participate (the passive and homogeneous matter) is not the only one, as Diderot demonstrates. Working from the assumption that matter as true substance must be applied not only to technological

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<sup>33</sup> In France, Bachelard (*Le Matérialisme rationnel*. Paris: PUF, 1953) tried to think materialism from a chemical point of view. But this interesting book considers materialism in a very restrictive meaning (theory of matter) and neglects the philosophical and classical materialisms. Thus, one would ask that the chemical point of view also envisages what is called materialism since the 17<sup>th</sup> century, with its specific issues (the origin and explanation of things with one substance, the materiality of explanatory agents and realities, etc.) and debates (the rejection of transcendent explanations, of the separation between body and soul, of the idea of a passive matter, etc.). The e-book, *Les Matérialismes et la chimie*, F. Pépin (ed), Paris, Editions Materiologiques ([www.materiologiques.com](http://www.materiologiques.com)), to be published in 2012, tries to revitalize the link between chemistry and the philosophical interrogation about materialism.

<sup>34</sup> “The Philosophy of Chemistry, From Infancy Toward Maturity”, p. 23-24.

<sup>35</sup> For instance in “La science au risque des matériaux”, *Cahiers philosophiques*, n° 85, décembre 2000, reissued in the *Cahiers philosophiques*, September 2006, p. 9-24.



productions, but also to an entire natural philosophy, it is interesting to compare with the link between “matters” and materials (*matières* and *matériaux*). Chemical philosophy has to deal with all natural substances and their transformations (natural or artificial ones). The issue becomes to consider matter or substance in a non-metaphysical point of view through its different kinds, its concrete transformations and qualities. Following Diderot’s example it is possible to interrogate on the one hand the similarities and the interactions between different substances (*matières*), and on the other hand the substantiation of qualities and forces. Three perspectives were articulated by Diderot; what might their relevance be today?

First, the dynamic relationship between different parts of heterogeneous substances represents a model of the *materiality of movement*, without simply stating that movement belongs to matter in general as several materialists did in the 17<sup>th</sup> and 18<sup>th</sup> century. Diderot proposes an investigation into the *production* of movement that remains independent of any exterior origins. This is a departure from the logic of rational mechanics where matter itself is considered passive because it is indifferent to its state of movement or rest and it is always set in motion by an external force. Diderot describes the graded differences from the physics of Descartes to that of Newton to chemistry:

There are philosophers so prolific as to have found sufficient explanations for all of the movements and the divisibility of a homogenous matter. But they are mistaken. How much easier would it have been if to these two principles they had added attraction, affinity, and the diversity of the five elements. And how much greater is the ease of those philosophers to whom the operations in the laboratory have taught them to recognise many other forces, actions and properties, etc.<sup>36</sup>.

Diderot proposes a specific form of materialism that articulates the pluralisation of “matières” and the attribution of the forces and qualities to matter. This places Diderot in direct opposition with the regularly renovated motif that insists upon the passive nature of matter that is then acted upon by an exterior force or intelligence. Is there still an opposition

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<sup>36</sup> *Observations sur Hemsterhuis*, p. 727. “Il y a des philosophes qui ont trouvé assez de fécondité pour suffire à tous les phénomènes dans le mouvement et la divisibilité d’une matière homogène. Mais ils se trompaient. Combien n’auraient-ils pas été plus à leur aise, si à ces deux principes ils avaient ajouté l’attraction, les affinités et cinq éléments divers. Et combien ne sont pas encore plus à leur aise les philosophes à qui les opérations du laboratoire ont appris à reconnaître beaucoup d’autres forces, actions, propriétés, etc.”

in that regard to mechanics and physics more generally? Most likely there is not, but these debates are again coming to the forefront as cybernetic models and nanotechnologies are developed<sup>37</sup>. Indeed, there is still a distinction between a representation of movement or information ignoring their material background, and a scientific and philosophical practice dealing with the materiality of forces. Diderot paints a perspective that is specifically chemical, describing himself as “one who deduces movement within materials (*des matières*), from their heterogeneity<sup>38</sup>.” This is an original version of the general idea of a relational ontology defining movement as the result of the rapport between different elements. This perspective also circumvents the direct opposition between the reality of objects and the phenomenalization of their interrelations, that is to say substances and reactions. There are several substances and they cannot be dissociated, even conceptually, from their properties. Matter is always in flux, intertwined with reaction.

Secondly, Diderot guards against any return to finalism in the interpretation of nature, this leads him to delve into the state of technico-scientific productions with great precision. For example, the concept of defining a function for a given material, whilst pertinent in the frame of a given technical project, is problematic for nature. In this case the concept of matters (*matières*) allows for the plurality of the substances within themselves and permits the conception, whilst avoiding finalism, of the interaction between their different properties and their effects. But there remains a problem: how to take orchestrate the architecture of substances, the most functional dimension of materials? This would call for technical models reducing function to its imminent effect in the interplay between different materials. Certain modern analyses looking at the role of processes in manufacturing seem to take on the methods of Diderot with their constraints singularities and fecundity<sup>39</sup>. But this problem merits a fresh philosophical inquiry, something that to date has been found nearly exclusively to evolutionary biology, and would deserve attention in philosophy of chemistry.

Thirdly, Diderot was amongst the pioneers to envisage a natural history of substances and what we now call materials. This allowed natural and technical determinations to come together under the flag of chemistry.

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<sup>37</sup> See B. Bensaude-Vincent. (2004). *Se libérer de la matière ? Fantômes autour des nouvelles technologies*. Paris: INRA Editions, in particular p. 51-54.

<sup>38</sup> *Principes philosophiques*, p. 399.

<sup>39</sup> For instance, see the analysis of Bensaude-Vincent (*Se libérer de la matière?*) and the one of François Dagognet (*Rematérialiser*. Paris: Vrin, 1989, in particular chapter IV).

Diderot anchors this natural history in a double perspective: descriptions of variety and transformations, thus allowing for a *natural* history as well as a technical one. Steel provides an excellent example<sup>40</sup>. Never found in nature it may nonetheless be produced from nature following a series of controlled operations. In this context steel may be seen as a synergy between nature and the *arts et métiers*; the furnaces may be employed artfully to reveal *full* nature of the elements in before us.

This leads to a question regarding philosophy of chemistry today: does it remain a philosophy of nature? Or is it foremost a philosophy of technique, a *phénoménotechnique*, as it is called by Bachelard? Masked behind this query is the debate about man's place in nature and our perception of science and its applications. Diderot presents a strikingly modern alternative in balancing a valorisation of technological advances and those that execute them whilst remaining humble before the infinite complexity of nature. This is a philosophy in direct opposition with the philosophies of the subject that affirm the power of man to harness nature. In its opposition it presents a conception where man and technology remain a part of nature, human beings are never an "empire within an empire" to paraphrase Spinoza. This attitude illustrates another debate in the philosophy of chemistry: does the culture and imagination of chemists stem from their subjugation of nature (the classical schema employed by philosophers working from the point of view of the physicist), or rather a humble practice echoing the *tâtonnement* of the artisan? The interface between the vision of chemistry, the philosophy of knowledge and anthropology is of the utmost importance here. It permits Diderot to radically reject the philosophers of subject such as Descartes (*a fortiori* the dualism between mind and matter) and contest the innate superiority of human beings as accorded by many diverse traditions. From this standpoint Diderot promoted technological progress epistemologically, philosophically and before society whilst rejecting the hubris of imagining man to be omnipotent before the passive matter of the universe surrounding us<sup>41</sup>.

## Conclusion

How might Diderot's work in chemistry remain of interest today? It represents more than the history of ideas. The time lapsed provides us the hindsight necessary to clarify our own philosophical debates from which

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<sup>40</sup> See the article "Acier" (Steel) of the *Encyclopedia* (article written by Diderot).

<sup>41</sup> See F. Pépin. (2012). *La Philosophie expérimentale de Diderot et la chimie. Philosophie, sciences et arts*. Paris: Classiques Garnier.

two questions in the philosophy of chemistry come to light. First, are there issues and types of analysis that are specifically characteristic to a philosophy founded on the viewpoint of the chemist? Diderot's philosophical inquiries and their subsequent demonstration via chemistry invite a broad historical viewpoint. Might this perspective reveal different *styles* of inquiry rather than eternal questions? Diderot has created one such style, through the optic of chemistry, as practised in by chemists in the laboratory. Second, how is it that this dialogue between chemists and philosophers often one in the same person took place during the Enlightenment? The strong presence of sciences in the eighteenth century's society and the interchange between people of radically different formations might have been a cause. This highlights once again the question of where chemistry takes place: the demonstrations in the *Jardin des plantes*, the *Encyclopaedia* and the accounts of the Royal Academia of Sciences of Paris all gave a remarkable publicity to this experimental science. But for Diderot, his passion for chemistry was driven by a philosophical reason: the elaboration of his experimental philosophy led him naturally to chemistry.

# SOCIAL DYNAMICS OF SCIENCE IN THE MAKING

BAPTISTE VOILLEQUIN

What is the History of Sciences and Technologies? Is it History focused on a specific social field, science or industry, or is it a chronological approach of sciences mainly dedicated to the education and collective memory of scientists? Is the term “History” meaningful enough to describe the diversity of tools and approaches necessary to analyze the scientific social field and the scientific knowledge production in a given historical context? How is a technical know-how developed and transmitted?

My approach is definitely multidisciplinary, at the crossroads of anthropology, ethnology, sociology, history and epistemology. It focuses on the study of the interactions between social actors and aims at understanding how knowledge or scientific objects (either an instrumental, material or conceptual one) emerge in such social environments.

There is no right word in French to describe this multiplicity of approaches. On the contrary, the English term “Science Studies” is well adapted because it suggests that human beings are at the heart of knowledge production, and it also creates a place where both Sciences and Human Sciences communities meet.

The History of scientific ideas is clearly insufficient. Scientific ideas, concepts, facts and know-hows have to be considered as products of scientists located in various social contexts and environments, in locations where knowledge is produced. The mechanisms of knowledge production can only be understood through the reconstruction of those social environments by analyzing the close interrelations between scientific concepts, approaches, uses, practices and politics.

My conviction is that men and women are the heart of knowledge production. That is why I consider that the methodology of Science Studies must focus on a close observation and analysis of the very daily scientific acts, uses, habits, behaviors and feelings. To understand scientists in action and science in the making, one has to undergo this

ambitious approach, consisting in catching punctual facts of so different types. This approach is based on immersing within research laboratories, industry and technology sites but also all other locations where scientific knowledge can emerge. Every location has its own specificities and will give birth to specific scientific knowledge and know-hows. Research laboratories, industrial development centers, industrial production sites, museums, classrooms, exhibitions, but also streets, archeological sites, agriculture fields, forests... are all locations that show true potential for science to emerge. Those locations are not only of geographical nature, they are also “social sites” meaning that they are also located within an institutional landscape, built by professional scientists, amateur scientists, politicians, citizens and shaped by local and global science and industry policies, but also broadly speaking by economy and culture. All those locations have an impact both on the nature of the scientific knowledge and on the mechanisms by which it emerges.

In addition to focusing on men and women of science, campaigns of immersion into laboratories will also focus on instrumentation, as the tools used in science can provide fruitful and rich case studies to understand in more details the production of scientific knowledge and the nature of a scientific and technical know-how. Several fields of science and technology generally need to be mastered to be able to conceive, manufacture and use those tools: for instance, a scanning tunneling microscope image is in fact an image rebuilt thanks to specific scientific concepts, signal treatment needs a scientific and technical knowledge about the nature and the meaning of each signal. Instrumentation is therefore implicitly full of knowledge of a certain kind that Science studies call tacit knowledge.

Technical and scientific equipment is a social object of many aspects: it is sometimes the fruit of great investment on behalf of scientific teams and it is the material proof of their effort, time, and of technical and scientific advances. Equipment is also quite expensive and is therefore the result of financial arbitrages that shape the life and practices of laboratories. In addition, the purchase, use and maintenance of such tools greatly influence scientific practice. This can be explained by several reasons.

First of all, scientists will have great expectations with regards to the results produced by the tools used, in order to legitimate such investments. Scientists will also tend to use the equipment extensively and to refer as often as possible to its use. The impact on knowledge production is not only quantitative but also qualitative. Whatever its motivations, a research team characterizing every sample by a new X-Ray tomography technique

will necessarily produce some scientific knowledge oriented on bulk material structure. And after a period of time and of assimilation, scientists of this lab will develop a specific vision on the structure of materials whereas a second team, who, by the same mechanism, will be focusing on an AFM technique and consequently develop a different conception of materials.

Moreover and secondly, the budget aspect of this phenomenon is often amplified by a spiral of cost. Huge investment costs lead to huge upgrading costs in order to avoid a too rapid obsolescence of the tool, which would be unacceptable in today's scientific world where up-to-date equipment is considered as a necessary condition for science excellence and fame. This correlation is so close that I have introduced the concept of amplifying "spiral of equipment". Such a spiral leads to over-instrumentation of some laboratories and can cause a unbalance in funding policies-when some funding are thought to be necessary and separate from global funding to be distributed by Research agencies, universities or companies-and can also cause the focus of scientific attention to drift away from research. The case of the French "Institut de Recherches sur la Catalyse" is a meaningful example described in my PhD-thesis.

I insist on this notion of amplifying spiral not because the impacts of instrumentation on science policy and science knowledge production, specifically in Physics and Chemistry since WWII, have not been well studied and described but because this phenomenon shows very well how knowledge emerges in a specific environment, understood as an ecological context where many forces interact resulting in a local social equilibrium. It shows how difficult and how long it can be to modify this environment and how strong the forces must be to change a given situation and context. And such historical situations are fruitful cases for analyzing the forces resulting in a context on which the production of knowledge occurs. Coming back to the case of the French IRC, the "spiral of equipment" underlines how the macrohistorical context-French policy to develop a strong science excellence and the general evolution of research in the field of chemistry since WWII with the introduction of many physical characterization methods-the national policies -creation of strongly supported CNRS Research Institutes very well equipped-local policies-strong support of Lyon to maintain its chemical industry-human factors-the vision of Marcel Prettre, its founder and first director-and scientific factors -up-to-date characterization of catalysts-interact and are intrinsically linked when speaking about knowledge production.

Knowledge production locations are also places where men-and women-of science live, develop and evolve. Observing their practice

cannot be enough: this approach needs to be completed by many other approaches, among which is capturing and understanding the perception that scientists have of their own activity. During oral investigations, it is particularly important to listen and, let's insist, to hear, scientists without any *a priori* assumption, betting on their honesty. Then, the distortion between the perception of a scientist and a situation needs to be analyzed in order to enrich and reappraise the considered situation. Thus, orally interviewing scientists is the second methodological tool that completes the previous approach. For instance, when every member of the French community of research on catalysis has underlined the historical role of Paul Sabatier considering him as the founder of modern catalysis, whereas historical data and international analyses prove otherwise, it enables us to understand both the importance of the process of the construction of a mythic founding father for research communities and more generally speaking the importance of memory in the social legitimation and social structuring of scientific communities.

Archives and other written non-scientific data (such as official or personal reports, meeting minutes, project files...) are very important sources to feed this multi-dimensional and multi-analytical approach of considering the mechanism of knowledge production and the processes by which scientific objects emerge. There is no denying that official archives have always been intentionally written. A scientific project can easily be associated to a political one: its aim is indeed to reach identified readers such as funding evaluation committees. But rather than neglecting such official written sources, one can fruitfully analyze them to compare sources and versions of some similar historical events or situations to use them to understand given past political contexts. Because by analyzing the criteria on which the submitter has paid attention to, we gain access to what he was then considering as the evaluation criteria and the expectations of given committees.

Often considered by scientists as a waste of time, not strictly necessary to the production of knowledge, the fact that a given scientist or a given team makes this effort is by itself an important fact that has to be considered: is the report considered by the writer compulsory for recognition by the peers or the policy makers, for visibility within the community, for funding, for gathering teams or communities, for addressing a challenging issue?

In addition one must underline the fact that the recent period has been marked by the importance of science policy on the international political scene since WWII. Since then, science and technology development have been considered by policy-makers as a key parameter of competition



between countries and between Western and Eastern blocs. The Vannevar Bush report published in 1945 marks the great emphasis put since then on science policy (Bush 1945). From then on science is conceived on a positivist vision of human progress; science is a good that can be put under control and scientific research as industrial development can be programmed.

In such a context where science policy has become predominant, one can understand that the self-positioning of scientists has been deeply reshaped. A strong science policy will shape the priorities of fields of research, trigger off specified rules for financing and advocate or even dictate research plans. The production of knowledge is even more affected when produced within a project, as scientists tend to fit their work to the rules and the expectation of selection committees.

This leads us up to question the way we can describe these deep macro-historical mutations and the impact on science and technology. The notion of regimes of knowledge production has been fruitfully introduced.

The early seventies were a period of deep upheaval in western societies. Analyzing the deep mutations that occurred then is a meaningful way to demonstrate how the long-term evolution of scientific and technological knowledge production can be tackled. Both the social crisis of 1968 and the oil crisis of 1973 are very significant symbols of the dynamic of huge mutations. At the time, a large public debate was launched to study how institutional systems could materialize and could take into account these mutations. One of the central questions raised in France was whether to open the academic research organism, the CNRS, to other research organisms and to other research modes than centralized directed research. The concept of "Associated Laboratories", gathering both CNRS and university researchers was thus created in the mid-sixties, opening the CNRS to the academic world and solutions were found to shorten the gap between academic research and industry. The idea raised from this public debate between 1972 and 1975 is that knowledge emerges from the confrontation of various points of view, competencies, know-hows and disciplines. Many institutions were set-up to stimulate these confrontations, and led to the creation of the RCP, CNRS ATP and DGRST AC and, later, GRECO (RCP: "Recherches coopératives sur programme". ATP: "Action Thématique sur Programme", AC: "Action Concertée"; GRECO: "Groupement de Recherches Coordonnées"). But this is not an easy task to select the best domains of research adapted for converging interests and for very different competencies: they are called "transfer sciences". Chemistry but also more specifically catalysis have been paradigmatic cases of "transfer sciences".

Highlighted as a “transfer science” through the emergence of the new regime of knowledge production, catalysis itself deeply changed. First, since 1973, catalysis has evolved from being merely a means of making money, to a way to optimize energy. In a second step, a new dynamic appeared with the emergence of environmental catalysis, highlighting catalysis as a means of minimizing the impacts on environment. We can see here an important aspect of the occurring changes. “Transfer sciences” like catalysis need an important additional feature: they need to be directly linked to political and social issues. This paves the way to a new type of research based on multidisciplinary programs and aimed at addressing social issues.

The early 90s also brought change to the regime of research. For a while, a multidisciplinary work seemed to be guaranteed. The reasoning is that multi-disciplinary is based on the excellence of each contributor. Thus, excellence was defined as the new priority.

But the question was then to know how to make excellence a priority without moderating interdisciplinary incentives while keeping contact with social and political issues. The solution has emerged clearly: excellence will come from high-tech instrumentation. “Excellence hubs”, called “pôles d'excellence” in French, that were created in the late 90's are organized around research and innovative regional centers based on shared instrumentation. For instance, from the “Lyon catalysis hub” that was created in the late nineties emerged the project of a common NMR-center and has led to the creation in 2005 of the very high field-NMR center (CNMR).

Such a system based on centers of excellence is an organic one: local and national institutions support material needs, equipment and pay scientists; Europe gives the strategic roadmap by defining programs and by financing projects corresponding to those programs.

This new pragmatic and utilitarian doctrine of excellence deeply modifies mechanisms of production of knowledge: knowledge is acquired by making. The proof is given by showing that nature is under control and that nature can be tuned to scientists' expectations. To come back to the example of catalysis, how could you better demonstrate that you know what adsorption on metal really is than by showing, as the 2007 Nobel Prize of Chemistry Gerard Ertl did, that you can control and balance competition between molecular adsorption of CO and O<sub>2</sub> on Pt metal surface. Synthesis and making of catalysts is still not only a preparation step necessary use active materials, but is fully integrated in the scientific process of making the proof and acquiring understanding and knowledge on catalysis.

Proof has been made that academic categories considered as disciplines, research specialties, or research schools are more than confining political boxes but are important categories that not only liberate but also organize and classify knowledge. Understanding the historical mechanism by which these mental maps reshape the institutions is extremely fruitful for science studies. From a research topic to a discipline, the mental object becomes a social institution by being socially constructed by scientists, policy-makers and even citizen. How does a specific scientific topic become first a specialty for a couple of scientists, and then an academic social field sufficiently recognized as independent and consistent to educate students, to offer jobs and careers? How can this knowledge be considered in the end as sufficiently important to be taught to youngsters as founding elements of understanding for every citizen? These are important questions to be answered. The process of this mechanism, by which a mental map is changed into an institutional reality, can be identified by key labels that can help to define the notion of discipline. The case of the emergence of catalysis in France—but throughout the world with some national specificities—is typical.

The first meetings of the community of research (Lyon in 1949, Liverpool in 1950) have paved the way to the first international meetings considered as such (Philadelphia in 1956 and Paris 1960); associations (North American Catalysis Society) and specialized papers (Advances in Catalysis published since 1958 and the Journal of Catalysis appeared in 1962) have been founded; dedicated laboratories (Institut de Recherches sur la Catalyse in France in 1958, the Boreskov Institute of Catalysis in Novosibirsk in 1960 and the Sapporo Institute on Catalysis) are set-up; teaching courses are included in the curriculum of the School of Engineering since the mid-sixties, and dedicated books are published: in France, the first book published for the general public was “Catalysis and catalysts” published in 1947 by Marcel Prettre and edited by “Que sais-je?” series (The literal translation of “Que sais-je?” could be: “What do I know?”). Later, the publication of the first textbook monography “Heterogeneous Catalysis” written by Jean-Eugène Germain in 1960 shows that catalysis has become a discipline in its full educational dimension at that time.

Simultaneously, the boundaries of the establishing discipline are claimed by the members of the international community. Once more, I insist on the fact that men and women are behind these categories, these socio-political structures. But the history of the institutional object “discipline” seems too uniform and too unified. Undoubtedly, case studies show that the historical reality is quite different. Divergence, debates,

alternatives, split but also compromises, consensus and convergence are all realities. Arguably, the notion of “research school” or research communities integrates well the disparities within the dynamics of the social field of scientific research. And furthermore, these notions are the transcription at the scale of social actor and social group of what the notion of “discipline” is at the political and structural scale. Research is definitely not an isolated act. As Ludwik Fleck explains: “the cognitive act is the social act par excellence”. It is idle to claim that an isolated man could even formulate a concept! The notion defined by Fleck is efficient: he introduces the notion of “collective thought” (The German term of Fleck is “denkkollektiv”). Every scientist is a member of a group, is located on a given context and he produces knowledge explicitly and implicitly as a member of this environment. This notion of “collective thought” translates socially the importance of the location where knowledge is produced. As ecological niches, these locations are geographical, social and scientific nests from where specific scientific knowledge or even “cognitive styles” (Fleck term) emerge (Fleck 1935).

This notion of “collective thought” has contributed to spread a positive meaning of the concept of “research school”. The term “research school” first appeared with a negative meaning: it was referring to historical cases of isolated centers under the patronage of a powerful and dominating master where scientific research was restrained and where innovation and the emergence of new ideas was consequently limited. But since the seventies, a positive meaning of this concept has been fruitfully developed: a research school grows institutionally under academic context (university, research institutes...), it is embodied by teachers and students, based on working methods and thought styles, preferred ways and tools to spread the “doctrine” and ways of thinking, and key masters that symbolizes it. Once more, this concept shows how important the location impacts on the production of knowledge.

During the process of development of catalysis as a discipline in France, three independent research schools have emerged. Each of them can be portrayed:

First, the *Prettre research school* flourished in Lyon, the French Manchester, with the unconditional support of the CNRS. There, many students of the chemistry Institute of Technology, called ESCIL, and of the University of Chemistry have been taught by Marcel Prettre, while many of them have become members of the *Prettre research school*. In the very aftermath of WWII when French science had to be utterly rebuilt, the CNRS had first chosen the team of Marcel Prettre to develop research on catalysis. A few years later, in 1958, the foundation of the “Research

Institute on Catalysis” (IRC) was simultaneously a proof of national recognition and of international fame of the *Prettre research school*. The excellence and expertise of the IRC on up-to-date characterization of solid catalysts was internationally well known. Based on such an expertise, the Prettre research school has been leader on developing the electronic theory of catalysis during the sixties with the Boreskov Russian school of research. Under the electronic theory of catalysis, the catalytic act is described by the electronic states of the catalytic solid. Between 1958 and the late seventies, basement of the *Prettre research school*, the IRC was not the Research Institute on Catalysis but the Research Institute for Catalysts...

The *IFP research school* has emerged within the public Oil French Institute (Institut Français du Pétrole) created in 1945 to support the development of the French oil industry from exploration to the pump. To rapidly construct a strong expertise from scratch, the high management of the IFP involved a very famous Belgian master, Joseph Jungers, trained at Louvain where he met Hugh Taylor during his stay there two years before WWII. Since 1958, young recruits can spend some time abroad to train in Louvain (from 3 to 6 years). With this strong institutional support and this efficient strategy for developing a new team of research, IFP was designated to organize the Second International Conference on Catalysis in Paris in 1960 Prettre was the President of the Scientific Committee, and Navarre, CEO of the IFP, was the President of the Organization Committee. After this event, the IFP research school has been integrated at the international community. In line with the general mission of the IFP and explicitly presented in the influential “*Cinétique chimique appliquée*” published by Jungers and al., the *IFP research school* advocates a specific vision on catalysis. The objective for a modern catalysis is to aim first a precise knowledge of chemical kinetics to control industrial chemical processes. The fact underlined is that chemical engineering cannot be efficient if the chemistry behind it is misunderstood. So kinetics are a determining factor for a modern chemical engineering.

The *German research school* was founded by Jean-Eugène Germain, former student of the École Normale Supérieure in Paris where he recruited two students, Raymond Maurel in 1951 and François Gault in 1952. After a year spent abroad with Herman Pines in the Ipatieff Lab at the Northwestern University, Germain, and consequently the raising team, moved to Lille. Lille became then the very “*berceau*” of the *Germain research school*. The immediate signature of an important collaboration contract with the French “*Houillères du Nord*” modeled the future close collaboration that the school has with industrial partners. After the

restructuration of the French university system labeled by the founding Conference of Caen in 1956, the *Germain research school* has taken advantage from the newly reaffirmed role of universities in French research system and from the foundation of many universities in the provinces. Raymond Maurel moved to Poitiers, François Gault moved to Caen and then to Strasbourg and set-up there *sister teams*, not only in close connection to the mother team in Lille but also in agreement with the research strategies, techniques, concepts, theories and style. Less directly supported by the CNRS, the Germain research school is strengthened by being in close relation with industries and by being deeply involved in university teaching system. The science of catalysis that has emerged is focused on the precise description and understanding of the kinetic mechanisms of the key industrial catalytic reactions. The “catalytic elementary act” is the central concept developed to describe the catalytic phenomena. Induction is preferred: with a broad precise knowledge of various catalytic reactions, the essence of the “catalytic act” is extracted. The cognitive scheme is as follows: describe the mechanism, decompose into elementary acts and then determine catalytic acts. Here, addressing key industrial reactions is a guaranty to be sure of studying in a certain extent more typical and canonic reactions, and to tackle the true issues of the science of catalysis. Within the Germain research school, the attention is not focused on catalysts nor on kinetics but on the elementary transformations of the chemical substances (reactants, products, reaction intermediates, but also by deductive analysis transition states). Preferred characterization techniques are for chemical analysis (mass spectrometry, chromatography techniques, spectroscopy techniques –IR, UV/visible, NMR-) and for isotopic analysis (deuterium and other heavier isotopes, topic on which François Gault built an international reputation). The main textbook defending this vision is the *Catalytic Conversion of Hydrocarbons* published by JE Germain in 1969, dedicated to Vladimir Ipatieff and prefaced by Herman Pines himself.

Each of these three distinct research schools have their own specific geographical locations, masters, institutional supports, their access to teaching and training organisms, their manuals and their textbooks, and their own vision on catalysis, their own cognitive styles on research. It is idle to emphasize once more the importance of the location where the knowledge is produced: the scientist is not isolated, he is trained, he has colleagues, he has his own style, and he has access to specific instrumentation.

When the history of disciplines is by definition a uniform positive story of success, the concepts of social groups as research communities or

research schools permit to address discrepancies and competition on dynamics of science.

At this point the issue of the social identity of the scientists is tackled. Legitimacy by memory is one of the key ways by which this identity is designed. Scientists don't wait for historians to build the history of their own disciplines and fields of research. Even if this history is different from academic history both by its aim and by its methods, this history is essential and efficient. That's why Science Studies have to analyze and understand precisely the history of this memory. This history is necessary to scientists: it contributes to define their own social identity. By its function, this memorial history is full of myths: commemorations and anniversaries are crucial events, and the founding father is untouchable. This founding father represents a given image of what the "son" referring to him wants to be associated to. One can understand that the aim here is not to develop a strict historian method but more to retain selected key aspects that can contribute to building the expected figure of the founding father. This mechanism is so fruitful for understanding science in the making!

There is no denying that Paul Sabatier can be considered as a major builder of modern catalysis. Awarded with the Nobel Prize in 1912, powerful dean of the University of Toulouse for years, Paul Sabatier became a key figure of French chemistry-and of French Science at a whole. Sabatier became a myth, as soon as 1929. Two main contributions are cited when referring to Sabatier. The first one is his crucial contribution of the understanding of the catalytic hydrogenation, and its impact on the modern processes of the hydrocarbon industry. Thus, Sabatier is considered by French chemists to be the founder of the modern oil industry. The second one is his theory introducing reaction intermediates into the catalytic mechanisms. Thus, the debate to know if catalytic action is a physical action or a chemical action is closed. A chemical reaction occurs between catalysts and reactants. These crucial works, its undoubted international fame and the personality of Sabatier have contributed to make Sabatier the founding father of the modern catalysis for French chemists.

All these elements tend to prove that Paul Sabatier is the founding father of modern catalysis. However the impression is completely different if one refers to Anglo-Saxon sources and papers where Sabatier is quoted among others, whereas other important figures are preferred. French perception of the historical role of Sabatier seems to be exaggerated. The question here is not to know if Sabatier is the true founder of catalysis or not or if its works on hydrogenation is the first step for catalytic cracking



or not. My objective is here to analyze the mechanism of mythology. This is a fact: since the end of the eighties, for French chemists, Sabatier has undoubtedly become the founder of modern catalysis.

Why has Sabatier been branded as the founder of catalysis? This phenomenon is rooted in the 1980's under the dynamics of gathering of the three research schools described above. As Barthes explains, the efficiency of a myth is to potentially many different meanings attached to it—let's say a great liability- depending on periods and on contexts (Barthes 1957). The myth of Sabatier took a new dimension in the nineties. First, the mythology of Sabatier had been extensively used to legitimate and symbolically rebuild the republican French science –and especially chemistry-on safe grounds after having been dangerously weakened during WWI. After the end of the eighties, through the myth of Sabatier, French catalysis regained the image of a unified community developed since the very beginning of the development of discipline catalysis. Symbol of a founding father of the modern catalysis, Sabatier embodies an internationally famous French community of catalysis that has lasted from the foundation of the research area. The French community of researchers on catalysis does not refer to Prettre or Germain but to Sabatier, all of them re-inventing common roots to be unified under a consensual cult.

For the newly unified French community of researchers on catalysis, Sabatier enables one to view the history of French catalysis as a linear storyline. French catalysis can be claimed to be one and to have always been one. By focusing the debate on Sabatier's legitimacy, every French researcher can agree. The myth is fully efficient. It is not only a symbol of reunification, but also a common value of unity and strength in which every member of the community is involved. This comes to show how the existence of this memory is essential to the equilibrium and stability of the scientific community, a social body made of men and women living in a social ecosystem.

Taking into account various approaches, disciplines, timescales, and geographies, this sociology is an efficient methodology and approach to understanding science and knowledge production in all its complexity and meaning. The multiplicity of locations where knowledge is produced requires us to think of a multiplicity of scientific objects. Here the crucial question of the relationship between academic research and industrial research emerges. And this question is particularly crucial for chemistry and even more for catalysis where industry has always been linked to research. Two types of misunderstandings have to be avoided. The first is to make no distinction between academic research and theoretical or fundamental science and similarly between industrial research and applied



science. It is idle to claim that each concept has to be well differentiated from the other: the first couple of terms refer to a social or institutional position where the science production occurs, whereas second refer to the nature of the knowledge produced, the methods used and the objectives of the research done. The second misunderstanding to be avoided is to think that academic research and industrial research are two strictly distinct worlds. The solutions require a combination of both of these extreme worlds. The same reasoning can be used for fundamental research and applied science.

One must pay attention in particular to these distinctions addressing the recent evolution of the regime of knowledge production. As we have already described, the regime of knowledge production has deeply evolved from the seventies with the first emergence of the issues of energy harvesting. The social function of science and technology transformed from a vector for progress to a vector for controlled progress. To address this huge challenge, many solutions were proposed. But the common characteristics of these various solutions were that attention was mainly paid to transverse and multi-discipline projects. Science, innovation and knowledge production was expected to emerge by gathering many various approaches and expertise. Under this new regime, new locations of knowledge production were settled, geographically speaking—shared instrumentation centers, competitive poles, excellence centers- and institutionally speaking —industry/university mixed research units, French CNRS/university labs...-. The most interesting point here is that these mutations have impacted the very nature of the knowledge produced. Science has changed. Research is no longer science as well as technology but clearly a hybrid called technoscience. Boundaries between traditional science and traditional technology have been blurred. Technique is so integrated to science that the first is the “natural environment” of the second, implying the gathering of both industry community and scientific community. This gathering is done in a context where social issues are defining the transverse projects. In the field of catalysis, the objectives are to control the emission of pollutant gases, to optimize the retreatment of wastewater, to develop alternative energies... And the involvement of public policies is essential: pollution norms, sulfur level norms for fuels...

Multidisciplinary, transverse, instrumented, utilitarian, and close to industry issues, catalysis is a typical technoscience. The term technoscience is sufficient to understand that the blend of science, techniques, politics, social, and economic issues does not necessary mean that every research is applied. The confusion between important dialectic terms mentioned

above in this paper—such as academic/industry and fundamental/applied—is then avoided.

My conviction is that science studies have to mix complementary approaches: oral interviews and written sources; national science policies and local institutional solutions for labs and research organisms; general politics and individual choices; local constraints, visionary research programs drivers and science production mechanisms; community synergies and intern differentiations.

Long-term periods have to be taken into account. Carefully, one will catch general drivers of the production of knowledge and describe regimes of production of knowledge.

This methodology for Science Studies based on an anthropological and social history and taking into account various scales of analysis and various types of understanding paves the way to investigate closely the knowledge produced and the nature of science objects, science products. Then, one can at this step of analysis tackle epistemology, questioning rationality, truth, proof and essence of nature.

I advocate a multidisciplinary approach for Science Studies, aware of different points of view and open to new concepts and methods. Only then can Humanities catch the impressive variety and wonderful interest of science alive. Only then can Humanities describe this historical social group made of men and women called scientists. Only then can Humanities understand the mechanism by which knowledge is produced.

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# AGRICULTURAL CHEMISTRY, AGRICULTURE AND WHAT WILL HAPPEN TO THE WORLD: CONSIDERING SWIFT, COMTE, BERTHELOT AND SOME OTHERS<sup>1</sup>

DOMINIQUE PÉCAUD

## Introduction

Eating satisfies a vital function that is necessary for human survival. Agriculture is one of the human activities serving this need. It uses the virtues of organic soil to grow plants for human food or feed for livestock. The term “mother earth”<sup>2</sup> describes the symbolic world in which human cultures<sup>3</sup> link natural elements, human activities and teleological beliefs.

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<sup>2</sup> The United Nations said that: "The proclamation of 22 April as International Mother Earth Day is an acknowledgement that the Earth and its ecosystems provide its inhabitants with life and sustenance. It also recognizes a collective responsibility, as called for in the 1992 Rio Declaration, to promote harmony with nature and the Earth to achieve a just balance among the economic, social and environmental needs of present and future generations of humanity." (www.un.org, accessed august 10, 2011).

<sup>3</sup> We will use the expression "traditional cultures" to refer to shared representations relating to life-world systems. These systems rely on different explanatory modes: beliefs, science. We will talk about holistic systems, to discuss the global aspects of different systems of representation. We oppose ‘traditional cultures’ to ‘scientific culture’, from the moment that ‘scientific culture’, for its development, rejects any ‘esoteric’ explanations (Comte, 1893, p. 229-230). Comte does not systematically reject the spontaneous explanations of traditional cultures. Sometimes, he believes, they deserve to be subjected to reason. So, concerning the definition of living organisms, he says: "The obvious inconvenience of using two distinct philosophical terms to designate a single concept makes one feel that, in order to avoid a deplorable degeneration of the highest scientific questions into puerile discussions of words, it is not less indispensable to restrain carefully the name of life solely for really living beings, that is to say organic, than to attribute to it an

However, the history of agriculture is not only the history of this idyllic link. It takes into account how humans have sought everywhere and probably always, especially using technology, to exceed the natural capacity of soils, plants and climates, and, in the modern era, to master agricultural production through the application of scientific knowledge. *Use of techniques*: for a long time, tools and technology have been used in agriculture in order to improve production and increase efficiency. *Application of sciences*: botany, genetics, mechanics and chemistry offer to farmers the opportunity to take into account vagaries of climate, to accelerate the growth cycle of plants and animals, to reduce plant and animal diseases. Agriculture has gradually changed from being a traditional activity to become an industry.

Industrial control provided by scientific applications is supposed to produce an activity with high productivity. It aims to guarantee predictable results. At the same time, any new hazard encountered is recognized as an intolerable danger. This is the paradox of industrial activity, from which modern agriculture is not exempt; the more a human activity is based on techniques considered safe, the more humans become susceptible to the emergence of hazards. Meanwhile, the further hazards disrupt control of the activity and the predictability of its results, the more humans strive to seek new solutions to increase anticipated productivity and control. But these solutions inevitably give rise to new hazards.

In the nineteenth century, chemistry has been an important source of scientific knowledge that has inspired inventions and applications: fertilizers, products to treat plant and animal diseases, protection against insects responsible for damage to crops. Much of this knowledge that has found applications in agriculture derives from the technology of war (e.g.: use of phosphorus in the manufacture of incendiary bombs or in the preparation of poison gas in the wars of 1914-18 and 1939-45)<sup>4</sup>.

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acceptance sufficiently wide to be applicable rigorously to all possible organisms and to all their modes of life. In this respect, as in relation to all really fundamental notions, philosophers would doubtless have gained much in treating with less disdain the coarse but judicious indications of popular good sense, true eternal departure point for all wise scientific speculation".(ibid)

<sup>4</sup> In 1854, French chemist Clermont synthesized the first compound of oxygen and phosphorus as base of nerve agents. In 1873, German chemist von Hofmann synthesized bases another nerve agent. In 1905, German chemist Haber produced liquid ammonia from the nitrogen of the atmosphere. In 1915, with Bosch, a German engineer, he built the first ammonia firm, to produce such toxic gases that will be used during the First World War. At the end of the war, the remaining stocks of these products were recycled as insecticides. Inspired by the work of von Clermont and Hofman, German chemist Schrader synthesized from insecticides,

This text has three parts.

The first parts comments on some writings of the chemist Berthelot to show the role of chemistry in the development of modern agriculture that breaks away from traditional farming practices. It has developed as the industrial mode dominant from the end of the nineteenth century. Adept of Scientism, Minister of Education and Fine arts<sup>5</sup>, Berthelot attributes to the “scientific law” the mission of guiding the future of humanity, and of dictating “moral conviction in universal solidarity”<sup>6</sup>.

The second part seeks to show how the positivist paradigm or, more generally, the scientific paradigm, while offering the Utopia of mastery of the world by Reason, introduced implicitly notions of hazard and accident, and reinforced the final rupture between man and nature. This paradigm also separated the human subject from the mineral, vegetable and animal environment at his service. Hazard and accident become signs of the imperfection of “scientific law” and denounce the lack of knowledge necessary to understand the world, and the lack of resources “to face up to it”<sup>7</sup>.

Finally the last part examines the present situation. It is marked by both the survival of the positivist project and by the desire for a reconciliation of man and nature. This reconciliation can go as far as to adopt radical solutions where man appears only as one element among others in the world (Naess, 2008; Afeissa, 2010). The applied sciences are subject to this duality. Originally at the service of man, they are now called upon to protect the environment, by prevention to end its degradation engendered by human activities, or, in reparation to restore the impaired state of the world. Can the applied sciences serve this reconciliation? This question leads to others: What 'Utopia' can provide this reconciliation? What new paradigm could be adopted for men to design together this 'Utopia'?

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respectively Tabun (1937), Sarin (1938), and Soman (1944). In 1949, an English chemist, GHOSH, working on the synthesis of pesticides, discovered VX, an extremely dangerous nerve agent (The V-series is the second family of nerve agents).

<sup>5</sup> December 11, 1886-May 30, 1887.

<sup>6</sup> "Science dominates everything: it alone offers permanent services. No man, no institution from today will have lasting authority, unless they conform to its teachings." (Berthelot, 1896, p. XI and XII)

<sup>7</sup> In France, a trade magazine for risk-prevention professionals is entitled "Face aux risques" (Facing up to Risks). This title illustrates the divide between men and an environment full of risks and naturalizes the concept of risk. (Pécaud, 2005)

## 1. Scientific Positivism and Agriculture

### 1.1. Scientific Positivism as the Culmination of the Extension of Applied Sciences

The end of the nineteenth century was marked by unprecedented expansion of industrial activities, and by domination of the paradigm of the alliance between Science and Reason. This domination was exerted on the set of human activities in order to serve universal progress.<sup>8</sup>

The experimental approach aims to establish causal relationships, limited in number but scientifically valid. These relationships permit the definition of stable 'natural' laws. Knowledge of the phenomenon and of its causal development offers the possibility of reproducing it. In technology, the application of these laws should rule out uncertainty. It must be possible to anticipate all outcomes. The philosophical and political project of Scientific Positivism leads to the extension of the experimental approach to all activities, including, where possible, human activities. The scope of understanding provided by the causal approach increased. However, at the same time, reductionism is a necessary requirement: experimentation can produce valid results only if based on known and controlled parameters. Solely respect of this requirement can guarantee validity. It is one of the conditions for predictability of results. The assertion "All other things being equal" is essential for the construction of scientific laws.

Yet the hope of an extensive knowledge of the world is not abandoned. Neither is the mastery of a world, defined in terms of the considerable resources it can offer to men, abandoned. Only three ways to progress are available to humanity: the extension of reason by increase in scientific knowledge; anthropocentric physical control of the world through applications of scientific knowledge; exploitation of the natural resources of the planet, or of the possibilities of substitution of natural resources by manufactured products, provided man has the energy<sup>9</sup> to do it.<sup>10</sup>

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<sup>8</sup> "It is only two and a half centuries since scientific method disengaged itself from all strange alloys and manifested its purity: its efficacy is attested in a great diversity of sectors, by unceasingly accelerated industrial and social development." (Berthelot, 1896, p. 3)

<sup>9</sup> In his criticism of the monarchy of Wilhelm II, Kracauer associates capitalism with veneration of energy. See: AGARD, O. (2010). *Kracauer, Le chiffonnier mélancolique*. Paris: CNRS Editions.

<sup>10</sup> "To speak of an energy source of heat or electricity, is to speak of a source of chemical energy. With such a source the manufacture of all chemical products

Agriculture is seen as a human activity, but it depends on the qualities of the soil on which it is practiced.<sup>11</sup> Berthelot defines two sets of useful elements to plants.<sup>12</sup>

Knowledge is being acquired, and recommendations are formulated. For example, in 1888, Berthelot and ANDRÉ published scientific research results on the determination of phosphorus and sulfur in plants in the *Journal de l'Agriculture* under the "Agricultural Chemistry" column.<sup>13</sup> de Gasparin acknowledges the value of these tests.<sup>14</sup>

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becomes easy and economical, at any time, in any place, at all points of the surface of the globe. It is in this that we will find the economic solution of the what is perhaps the greatest problem arising from chemistry, that of the fabrication of food products (...) Thus, the food problem, let us not forget, is a chemistry problem." (Berthelot, op. cit., p. 512)

<sup>11</sup> "Each plant demands (...) special elements and, to cultivate it, it is necessary either to ensure that the soil already contains them or supply them. Hence the utility, so long contested, of the chemical fertilizers: in them there dwells the secret of maintaining indefinitely the fertility of the earth and the whole art of intensive cultivation." (Berthelot, 1896, p. 142)

<sup>12</sup> "Some, such as oxygen, carbon extracted from carbonic acid, hydrogen from water, and, in certain proportion nitrogen from the air, are from the atmosphere which can provide them indefinitely. The others, such as ammonia, lime, silica, iron and in part nitrogen, are on the contrary extracted from the earth: drawn up by crops, they must be returned, to avoid a more or less rapid depletion. Each plant demands this return of specific elements: and to cultivate it one must either ensure that the soil already contains them or supply them." (Ibid.)

<sup>13</sup> "In the 'séance' of the Académie des Sciences on the 19<sup>th</sup> December, Messrs Berthelot and André presented a paper amounts of sulphur and phosphorus in plants, the earth and compost, and on their correct proportioning. According to Messrs. Berthelot and André, one cannot measure with certainty the total amount of phosphorus existing in the soil and in plants by known procedures, which only permit access to the mineral constituents and not the organic components in which phosphorus is incorporated." (*Journal de l'Agriculture*, agricultural chronical of 7 January 1888).

<sup>14</sup> "I interrupt the silence of my retirement to reassure completely the farmers and tell them that the analysis of Messrs. Berthelot et André are the full confirmation of the accuracy of the results we have given for the correct proportions of phosphoric acid, I should say, of total phosphorus, existing in arable land (...). No doubt it is otherwise for sulphur, which means that we do not allow it to them, and that they can count surely on that for phosphorus, which is for them of primary importance, given the enormous use of phosphates as complementary fertilizers." (*Journal de l'Agriculture*, idem)

## 1.2 Traditional Practice and Applied Sciences

During the first half of the eighteenth century, in the third book of *Gulliver's Travels*, Swift describes scientific projects concerning transformation of nature and traditional agricultural practices and criticizes them. In his preface to the translation of Swift's book, Tadié (1997) recalled that most of these projects draw their sources in the *Cinquième livre*, the book in which Rabelais (1995) described the existence of Kingdom of the *Quinte Essence*, or *Entelechy*.

During one of his travels, Gulliver visits the Great Academy of Inventors of Lagado, capital of Balnibarbi. "In these colleges the professors contrive new rules and methods of agriculture and building, and new instruments, and tools for all trades and manufactures; whereby, as they undertake, one man shall do the work of ten (...)", says Swift.<sup>15</sup> Gulliver meets a man. This man says him that: "He has been eight years upon a project for extracting sunbeams out of cucumbers, which were to be put in phials hermetically sealed, and let out to warm the air in raw inclement summers."<sup>16</sup> Thus is posed the question of conservation of energy for the soil of plants, of its storage and re-use later if the need arises. If it is possible to retain solar energy, it is also possible to regulate temperatures required for the maturation of plants; it is then also possible to program when they can be consumed.

Another discovery: "In another apartment I was highly pleased with a projector who has found a device of ploughing the ground with hogs, to save the charges of ploughs, cattle, and labour."<sup>17</sup> This metaphor, already present in Rabelais explains the available energy necessary to realize agricultural works. The status of animals is central. Here, pigs are substituted for foxes under the yoke of labor. The question of the mastery of nature is raised. How to improve agricultural productivity by bringing in all available forces? If pigs search for food opening fields with their snouts, is it possible to use this aptitude more systematically to plow farming fields? Pollan (2006) will cite the example of an American farmer who finds it is efficient to permutate on one site beef cattle, chickens and crops to sustain profitable soil.

Gulliver meets another engineer. "The projector of this cell was the most ancient student of the academy (...) His employment (...) was an operation to reduce human excrement to original food, by separating the

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<sup>15</sup> (Swift, 1997, p. 221)

<sup>16</sup> Ibid, p. 224.

<sup>17</sup> Ibid, p. 226.



several parts, removing the tincture which it receives from the gall, making the odor exhale, and scumming off the saliva. He had a weekly allowance, from the society, of a vessel filled with human ordure, about the bigness of a Bristol barrel.”<sup>18</sup> This activity described by Swift illustrates relativity or lack of “stable borders”<sup>19</sup> between anthropological categories from which we implicitly build the way we see world in which we act: sacralization of the 'natural' cultural and legal status of animals and men, symbolic value or worthlessness of objects, activities, materials and substances.

### 1.3 The Benefits of Science

The above allusions feed a sharp criticism of the “utopia of the universal benefits of scientific knowledge” (Tadié, 1997, p. 28). We can add: they feed the Utopia of the inherent tendency for scientific knowledge and its applications to neglect the existence of traditional practice in the name of unequivocal knowledge. Such knowledge would be able to describe rational human activity, with the aim of improving, not only the increased productivity that it would permit, but also the well being of those who create or benefit from it. Radical utilitarianism (Bentham, 2011) and Scientific Positivism indirectly support this worldview.

This criticism does not consider the *a priori* effectiveness of traditional practices, except to specify of what kind it is. Mauss (1968, p. 371) defines technical activity as “traditional effective action”<sup>20</sup>. Technical activity is material and symbolical only when societies or less important human groups can identify and define it as a common technical activity. Such groups are defined either from a diachronic point of view (mutual influence of its members) or synchronously (knowledge transfer). A technical activity is effective when it achieves good results for those wishing to achieve them. Mauss showed that, as a trial, the efficacy implies a view of the world. Thus a presently accepted division of labor, namely: 1) designers or engineers, 2) manufacturing technicians, 3) operators, 4) users or consumers, but also 5) politicians and moralists. In this context, a technical activity will be considered effective if and only if all of these different social actors agree about its efficacy, if they produce

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<sup>18</sup> Ibid, p.225

<sup>19</sup> (Klemperer, 1996, p. 100)

<sup>20</sup> The text is: "I call technique an efficient traditional act (and you see that in this it differs from a magical, religious or symbolic act). It is necessary that it should be traditional and efficient. There is no technique and no transmission if there is no tradition."

collective judgments about its effectiveness. We add that the chosen efficacy participates in different forms of rationality. It not only favours *instrumental rationality* defined an objective fit established between an event and its cause (Pécaud, 2005).

Of course, the possibility of agreement about the efficacy of an event is rare, and scientific knowledge is not enough to impose this agreement. For example, the relation between the fatal effects of the implementation of asbestos thermal insulation on human health and environmental pollution has been questioned only with great difficulty in France. Added to disputes relating to scientific risk assessment were disputes as to the nature of economic and political relations between the industrial lobbies, whistleblowers and victims. Another example: the assessment of efficacy concerning an insecticide, DDT (dichloro-diphenyl-trichloroethane), was widely established in the necessary antivectorial campaign<sup>21</sup> to protect the health of populations. This could not resist the analysis of its major environmental effects, in its mass distribution, on different forms of life. As a last example: the controversy that arose from the 90s concerning endocrine disruptors, the assessment of the environmental pollution they cause and, in particular, their effect on human health, notably fertility<sup>22</sup>.

In the eighteenth century, Jonathan Swift adopts an ironic attitude towards any universalist pretensions of science and its applications. He describes an Academy gripped by certainties: valid knowledge is claimed to be universal. It leads to applications that can only be beneficial to humanity. This benefit is undeniable. These are the characteristics of a scientific Utopia. Through *Gulliver's Travels*, Swift describes human activities as they might be ideally. The efficacy of practical techniques does not arise from decision taken in a relative way, but solely from the scientific value of that which inspires them. The Utopia denounced by Swift describes a world without reference to geography. Only applied *knowledge* can be effective, *since everywhere will be considered equal*. To contest the results of applications would be to contest the universality of what inspired them, to question the refusal of any critical thinking that

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<sup>21</sup> "In its widest sense, the antivectorial campaign includes the fight and protection against haematophage arthropods, vectors of agents pathogenic for man and vertebrates, together with their surveillance. It includes the fight against living insects when they are potential vectors or when the nuisance becomes a problem of veterinary or public health." (Fontenille et al. (2009). *La lutte antivectorielle en France*. Marseille: IRD Éditions).

<sup>22</sup> "*Endocrine disruptors*" is used for the first time in the Wingspread Statement (1991). The purpose of this text was to focus on impaired sexual development of humans and animals caused by chemicals and their interactions in the environment.

characterizes any Utopia.

One hundred and fifty years later, Berthelot begins a speech before the Société Nationale d'Agriculture de France, of which he is president. He recalls, but only better to oppose it, Swift's criticism of the Academy of Lagado visited by Gulliver. He strongly emphasizes the "*benefits*" of *science* when devoted to improving the productivity of everything in general, and agriculture in particular.<sup>23</sup> Two years earlier, in a speech at the Banquet of the Chambre Syndicale of Chemical Products, Berthelot (1896, p. 508) outlines a possible perspective. The application of chemistry should bring to an end the uncertain future entailed by farming methods attached to traditional use of the soil. This means abandoning an activity whose results he considers unpredictable. In other words, Berthelot suggests the need to bring an end to random farming results. This eradication assumed full control of agriculture, informed implementation of relations between the elements assuring production: soil, plants, and animals. He adds to this list the sciences: mechanics, chemistry, and physiology.<sup>24</sup>

## 2. Mastery, Accident and Hazard

### 2.1. Reason as Incarnated in Science

Reason as incarnated in Science is supposed to provide, in a durable manner, knowledge considered valid. Scientific Positivism embraces this point of view. It offers three methods that are three paths: observation, experiment, comparison (when the latter is possible). This knowledge can be criticized or confirmed by the production of new knowledge.<sup>25</sup>

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<sup>23</sup> "The scientific agriculture is substituted more and more for traditional agriculture, and multiplies in unhopd for proportion the riches of nations." (Berthelot, 1896, p. 37-146)

<sup>24</sup> Emphasizing "this indissociable alliance between science and industry is characteristic of modern society", Berthelot states: "In those times (i.e., according to him, in the year 2000) there will no longer be agriculture, shepherds or laborers; the problems of existence by cultivation of the soil will have been eliminated by chemistry!" (Berthelot, 1896, p. 508)

<sup>25</sup> "Whatever opinion one adopts as to the origin of the of the earth's crust, one could, it seems to me, admit, in fact, as fairly plausible, although in no way susceptible of actual proof, at least the distribution necessarily nearly uniform of the divers elements, or at least that their abundance would be much less unequal, in the whole of the globe than appears to indicate up to now the exploration of its surface. (...) our mineralogical examination concerns at present, and could evidently never concern more, even supposing it complete, than the superficial

Surprising remarks that link the taking into account of the necessary contingency of scientific practice, the confrontation of this approach to the particular, and a world view ("consideration of universal history") based on the general, here the chemical components ("*elements*", "elementary substances" assumed to be equal "in abundance". The overall vision of the world that this consideration depicts seems necessary to justify the "the primary results of present chemical analysis", caught as they are in the contingent perimeter imposed by the scientific method which produces them. This is not an imaginary vision but a working hypothesis that will undoubtedly be confirmed by the accumulation of knowledge and broadening of its scope.<sup>26</sup>

It is within this reasoning dynamic that knowledge of the world according to "scientific law" continues historically, and that the dissemination of this knowledge contributes to the "*Ernünchterung*" or "disenchantment" of the world (Weber, 1959, p. 96). But, in an apparently paradoxical manner, it is also in this same dynamic that, if not hazards themselves, at least our perception of hazards increases; if not accidents, then what are so in our description of them. It is in the different production dynamic that accompanies that of scientific reasoning that the occurrence of hazards and accidents will disappear. Scientists, but also engineers, will

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layers of the globe, without us being able to presume as to the true composition of nearly the whole of its mass. Now, if, to the principle of the uniform distribution of elements, one wished to add that this uniformity must exist, not only in the whole of the earth, but also in particular at the surface, it would become immediately very precarious, and even extremely implausible, for one can easily, it seems to me, entertain many rational grounds for the necessary preponderance of certain elemental substances at the surface of our planet, while others would dominate, on the contrary, it's interior. Consider, on the one hand, that the rarest elements at the surface of the globe are also, in general, the heaviest, and on the other hand, that the most common are above all those which are combined in the composition of living bodies. This undeniable double relation, un-noticed until now, evidently tends, on the contrary to render conceivable as eminently natural a very unequal distribution of the divers elementary substances between the interior of the earth and its surface, some must have predominated in the interior so as to render the average density of the earth so much superior as it certainly is to that of the upper layers, and the indispensable preponderance of the others being no less evident for the extreme superficial solids, liquids and gases, where exclusively life had to develop. Thus, this consideration of natural history, when sufficiently deep, instead of throwing doubt on the primary results of present chemical analysis, shows rather a propensity to confirm them, at least on the whole." (Comte, 1893, p.66-67)

<sup>26</sup> "No law can be really explained except in our being able to make it fit into another more general." (Comte, *idem*, p. 92)

eventually find a plausible explanation for their appearance. They will propose corrective measures.

Knowledge applied to a too narrow field, insufficient results in terms of a world desired, these are two obstacles to their dissemination and appropriation. This may be the view of many scientists and their political supporters. At the same time, traditional explanations are ignored or, when they are invoked, are discarded without much consideration, in the name of the struggle against obscurantism and imaginations. However, they could nevertheless constitute an orientation of thought.<sup>27</sup>

The harmony of the world seems posed as an *a priori*. The experimenter seizes it and if successful, the advance of science will recognize its validity. In this context, hazard, or accident have several origins: 1) lack of scientific knowledge necessary to understand a phenomenon perceived as such; 2) lack of scientific knowledge necessary to guide human action capable of holding off the emergence of such phenomena; 3) the fact of not taking into account the potential applications of the sciences; 4) the "human factor" that includes all the forms of license Man will take with guidelines for action inspired by scientific knowledge. Hazards and accidents break with the supposed harmony of the world that science has adopted as a mission to explain and, possibly, to confirm. This is finally the Positivist point of view prevailing in the late nineteenth century.<sup>28</sup>

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<sup>27</sup> Thus, this curious proposal of Comte: "But, although some facts seem already to confirm the principal, eminently philosophical, of a certain necessary and general harmony between these two orders of properties, one can, it seems to me, affirm that, in no epoch, this harmony has been neither sufficiently nor explicitly revealed as to incite a an immediate exploration of the chemical character of each element. Thus, without pretention of a chimerical perfection, one should always regard as acquired, by so many repeated direct observations, the chemical studies of the various simple bodies. However, this great general base once derived from experiment, all the other chemical problems, despite their immense variety, should be susceptible of purely rational solutions, according to a small number of invariant laws, established by the true chemical genius for the various classes of combinations." (Comte, *idem*, p. 13-14)

<sup>28</sup> "As we were saying just now, chemistry is today everywhere, and it is not possible to be disinterested in its progress and transformations ( ... ) Among the numerous subjects that these include, we must insist on those relating to agricultural chemistry ; in this way these precisions are provided on fertilizers, fermentations, milk, organization of laboratories, nutrition of plants, plant extracts(essences), etc ( ... ) one even finds there practical recipes which will be useful in many circumstances." (Extracted from a note written by the *Journal de l'Agriculture* (mai 1888) to mark the release of the book by Émile Bouant,

The *Journal de l'Agriculture* was created in France in 1866. It is concerned in France with all questions of agricultural practice and science, rural legislation, political and social economy in relation to agriculture. Reading it shows often how to combine practical knowledge and scientific proposals. Certain of these are the subject of recommendations or appeasement when disputes between farmers and scientists come to light<sup>29</sup>. It is typically the case concerning the fight against mildew blight.<sup>30</sup>

Twenty-six years after this chronicle, Berthelot insists on the beneficent role of science when addressing the 'Société Nationale de l'Agriculture de France'.<sup>31</sup>

### 3. Neoscientism and/or a New Social Contract

Let us summarize. The harmony of the world understood as the balance of its component elements nourished the background Scientific Positivism. The accumulation of knowledge, its development and expansion, should finally account for the validity of this hypothesis. This is what is suggested by Comte. But beware: no fanciful production referring to a lost origin, or teleological intention feed this hypothesis. Applied sciences, legitimized by the pure sciences, assume the mission of organizing human activity and of providing for humanity the benefits of a rational and protective order. If hazards or accidents occur, this means at least two things. Firstly, if the harmonious composition of the world remains an acceptable hypothesis, a sort of realistic route map, for the pure

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*Nouveau dictionnaire de chimie*. Paris: Baillères et fils).

<sup>29</sup> Fungal disease affecting the vine was caused by *Uncinula necator*: A parasite observed by Miles Joseph Berkeley in 1845.

<sup>30</sup> "We have recommended making trials, during the season 1887, of five formulas (...) the experiment last year fully confirmed our predictions, and before saying to which of these five formulas we finally accord our preference, it is suitable to recall at this time that scientists and winegrowers are not agreed, not only on the currently most efficient procedure against mildew, but also on the state or level of solution under which copper should be applied to the surface of the leaves. Our opinion, in this respect, presented in a brochure 'Mildew and its treatment and with numerous experiments in support in a memorandum' addressed to the National Society of Farmers of France, is well established." (idem)

<sup>31</sup> "General opinion has changed: the benefits of science have been so great, and they have transformed society in the XIX century so well, that no one would dare today to use the ironic language of the author of Gulliver. In truth I don't know but our great-nephews might succeed one day, by some artifice, in regulating the seasons (...) the innovations, criticized so bitterly by the English humorist, tend, in our day, to become routine in farm work." (Berthelot, op. cit., p. 138-139)

scientists, the applied sciences are confronted by a disordered world as soon as so-called common or ordinary explanations inspired by traditional culture are rejected. Hazards and accidents bear witness to this disordered world. The interpretation of their emergence feeds a culture of justification, which attributes to them a divided meaning. The applied sciences then propose technical solutions expected to put an end to more traditional ways of doing things. Solutions are implemented. Hazards and accidents appear as symptoms that arise either from the inadequacy of proposed solutions, from the incompetence of those implement them, or from the diversity of situations in which they operate. This last assumption recalls the judgment made on chemistry by Comte.<sup>32</sup>

Men will therefore develop new knowledge, conceiving methods of action, developing ways of organizing, to prevent the occurrence of adverse and unexpected events. Followers of a rational view of the world, scientists and engineers will, for example, conduct operational reviews to produce a scientifically valid explanation of hazards or accidents. They will submit their analysis to instrumental reason to understand and to prevent recurrence. They will reject the ordinary explanations belonging to traditional cultures (Pécaud, 2010). They will seek to impose the bringing together of new forms of knowledge and practice and will impose them in the reductionist approach as required by instrumental reasoning.

From the late nineteenth century, Berthelot has been the champion of a world that seeks to be rational and to break with more traditional views. Control and predictability of agricultural production must pass through a tearing out of traditional farming practices. Production of food is the sole target. Agriculture must not be allowed to continue as a holistic response to various functions such as a respect for traditional practices or a symbolic relationship with nature, notion itself embedded in a historical and cultural dimension. According to Berthelot, given the evolution of science, agricultural production should no longer derive only from chemistry. It is controllable at two levels. Chemical science applies to what Berthelot calls “chemical energy”, that is to say to all elements that

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<sup>32</sup> "(...) it is clear that, in most of its research, present-day chemistry hardly merits being called a real science, because it almost never leads to real and certain predictability. On introducing, into already well-explored chemical reactions, some defined modifications, even slight and small in number, it is rarely possible to predict accurately the changes that they should produce: moreover, without this indispensable condition, as I have frequently established in this treaty, there exists, strictly speaking, no science ; there is only erudition, whatever the importance and multiplicity of the facts collected. To think otherwise is to mistake a career for an edifice." (Comte, op. cit., p.4)

can improve agricultural production; this chemical energy itself arising from mastery of 'the eye of the needle' ('heat or electrical energy').

Berthelot assigns to chemistry a mission using a causal paradigm to serve a purely utilitarian vision of life in society. As noted above: science divorced from tradition is put to serve a world oriented toward harmony. This is one of the facets of human progress. The view we have of it is ambivalent: on one hand, we rely on valid analytical knowledge to formulate directions for action, because we are persuaded of their heuristic merit and ability to predict results as planned. On the other, we see unintended consequences of these actions when they interact with the environment in which they are deployed. We then analyze these results with similar analytical methods, seeking "corrective actions" as they are called in engineering language. Thus, the quality of causal reasoning, disturbed by observation of counter-intuitive effects, is reaffirmed in this quest for progress.

If farming practices arising from applied scientific agricultural chemistry dominate, it is not only due to the science that inspires them, but also to a number of different circumstances<sup>33</sup> including industrial, economic or symbolic power relationships, weight of institutions, and collusion of political and military perspectives. On the one hand, a "positive conceptions of causal links", to which agricultural chemistry is attached, participates in fact in a developing autonomy of logics of agricultural activities, ignoring on principle immediate or long term counter-intuitive effects of these logics. Thus, Berthelot foresees the disappearance of farmers within a century, but also on one hand the invention of a "spiritual chemistry which changes the moral nature of man as profoundly as our chemistry transforms material nature"; on the other hand, the fact of empowerment of chemistry is anticipated to inspire rational practices from this point of view, without rational analysis of the situational complexity in which these latter take place.

Where are we today? Berthelot's radical Scientific Positivism faces an historical evolution, the analysis of which calls for a paradigm of complexity rather than a causality paradigm. It seems that empowerment of science through the domination of instrumental rationality has not been achieved. Rather, it is rationalization of the world through the paradigm of causality that has progressed.

Consider two examples to illustrate this thesis. The first concerns the revelation of a counter-intuitive phenomenon related to the practice of

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<sup>33</sup> F. Jullien (1996) refers to "*situational potential*". The sociology of translation is concerned with various interactions resulting from the dissemination of new knowledge, especially that with practical application.



chemistry and the development of its applications in the industrial era. A recent article published in *Nature* indicates that POPs (Persistent Organic Pollutants) trapped since the beginning of the industrial era in the Arctic Ocean ice where low temperatures have favoured the deposition, now joins the atmosphere because of ice melting. In 2011, the extent of the dispersion shows that the efforts for two decades to reduce POPs presence in the environment are totally annihilated. The other example is the ban enacted in 2011 by EU about production and marketing of baby feeding bottles containing bisphenol A (BPA), a chemical used in the manufacture of plastic for food. This compound is now believed to have an adverse effect on the development of human body, increasing the risk of early puberty among women, reproductive abnormalities or adverse immune responses leading to the development of cancerous tumors. It is still in use in some electric kettles.

What can we learn from these examples?

The first suggests how the paradigm of complexity can provide possible explanations beyond apparent paradoxes, and may open new ways of solving environmental problems that we face. The situation that we have evoked had its source in the history of the chemical industry<sup>34</sup>, but is also exemplified in other dimensions such as global warming, which is generally agreed as being strongly induced by past and current industrial activities. Great consumer of chemicals, agricultural activity can certainly not ignore the role it plays in the impoverishment of soils and of the overall environment. This situation is not new. It is now the subject of preoccupation in our society. What justifications can we offer for intensive, agriculture, so-called *reasonable* agriculture, or organic agriculture? What feed the controversies on these different options? What is the energetic

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<sup>34</sup> Note that the chemical industry also provided substances that can transform the quality of life of vast territories. See how DDT and today larvicides of biological origin such as BTI (*Bacillus thuringiensis* subspecies *israelensis*), participate in the transformation of the living conditions of human populations. Invented in the late 1930s by Paul Muller of Geigy, DDT was developed and used to fight against mosquitoes transmitting malaria and typhus, but also as an agricultural insecticide. It was banned in the seventies, accused of being unsafe for human health. See: Pécaud D. (2010). "Mise en œuvre d'un projet interdisciplinaire en matière de prévention des risques sanitaires dans l'estuaire de la Loire: enjeux et méthodes", in *Sociétés Environnements Santé*, Vernazza-Licht N., Gruenais M.-É., Bley D. (dir.). Marseille: IRD Éditions, 35-60; Pécaud D. (2011). "Moustiques et territoire. Quand *Aedes caspius*, *Aedes detritus* et d'autres s'invitent en presqu'île guérandaise", *Espaces et sociétés*, 3, n° 146, 107-121. The programme ESTUAE (Entente des Sciences et des Techniques Utiles à l'Aménagement de l'Estuaire de la Loire) was financed by the Région of Pays-de-la-Loire (France).

state of the soil? Is it still possible to achieve the following two objectives: to guarantee global food supplies, to conserve soils and environments? Does this imply new forms of food, producing more locally what we consume, having a better distribution of wealth, and, more generally, to be mutually supportive?

The second example shows the growing importance of precautions taken to avoid unlimited chemical inventiveness in the service of industry and the economy. It also faces us with our contradictions. It shows us that while our responsibility is called for, its exercise is in practice limited, confronted as we are by dominant consumption standards.

Today, the hypothesis of going beyond radical Scientific Positivism that characterizes Berthelot's epistemological and political commitment, today remains fragile. Neopositivist thinking exists. For example, the relative success enjoyed by geo-engineering<sup>35</sup> maintains the hope of the applied sciences to overcome environmental challenges that we face. Supporters of this approach dangle the unlimited possibilities offered by technology enlightened by science. Thus nothing is really new. Was this not the illusion that Swift already described in order better to challenge it, and one that Berthelot sought to regild in the name of the great advance given by the science of his era? Physical control of the events on our planet is the object of large-scale technical protocols for which their inventors seek funding. More than a century ago Berthelot did not hesitate to promote human activity that could break the traditional contract between men and nature. However this contract is to be seen as regulation in the sense that Mauss (1925) evokes a mutual exchange between a "gift" and a "return-gift"<sup>36</sup>. This contract is also balanced in the sense that, on a symbolic level, what men take from or give to nature must be equivalent to what nature takes from or gives to men. For his part, Berthelot estimated that the power of chemistry did not have to worry about this relationship nor its equilibrium as, according to him, agriculture, like all human activities, is independent of nature.<sup>37</sup>

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<sup>35</sup> "All techniques aiming to stabilize the climate system by direct management of the energetic equilibrium of planet Earth by remedial reinforcement of the greenhouse effect". According to the definition of the French group "GIEC" (*Groupe d'Experts Intergouvernemental sur l'Évolution du Climat*). Site: [www.ipcc.ch](http://www.ipcc.ch), accessed august 10, 2011.

<sup>36</sup> In its own way, the current of thought of *Deep Ecology* (Naess, Afeissa) adopts this paradigm to review inherent rights and duties of members of a community of beings in nature.

<sup>37</sup> "On that day chemistry will have accomplished a radical revolution of which no-one can calculate the scope: there will no longer be neither fields covered with

The restorative scenarios suggested by scientists and engineers involved in geo-engineering research take up the torch for global industry. These are not only the anthropocentric elements of the world of human experience that are aimed at, those that Berthelot sought to denaturalize to escape the limiting constraints that traditional culture conceives, it is now the whole dynamic world that is concerned. Thus, it seems possible to transform climate impacts by implementing techniques that can redirect climatic phenomena of which the scale at which we perceive them led us to believe that their transformation were inaccessible.<sup>38</sup>

Finally, it is certainly a headlong race into the future that we are invited to join, voluntarily or not. In recent year *green chemistry* has shown an ambition to develop new processes and chemicals to eliminate, or at least reduce the physical, toxicological danger of substances or processes, some having been in use for a long time (Anastas, Warner, 1998; Lancaster, 2002). Its declared ambition is great: to maintain our lifestyle while modifying the industrial production that partly supports them. Another example: during a meeting<sup>39</sup>, Keith, a figure of reference in geo-engineering, considers the option of sending sulfates into the stratosphere, thus proposing a solution that to him seems effective and to hand to slow global warming.<sup>40</sup>

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harvest, nor vineyards, nor pastures covered with beasts. Man will gain in gentleness and morality, because he will cease to live by carnage and destruction of living creatures. There will be no longer distinction between fertile and sterile regions. Perhaps, even, the sandy deserts will become the preferred abodes of human civilizations, because they will be more salubrious than the poisoned alluvions or these marshy plains stuffed with putrefaction, which are today the seats of our agriculture." (Berthelot, 1896, p. 513-514)

<sup>38</sup> Swift, ironic: "There was an astronomer, who had undertaken to place a sun-dial upon the great weathercock on the town-hall taking into account the annual and diurnal motions of the Earth and Sun, so as to correct all accidental turnings of the wind" (Swift, op. cit., p. 227); or Berthelot, serious: "Truly, I don't know but our great nephew might one day by some artifice succeed in controlling the seasons: the Americans certainly claim today to be able to make rain when they wish, by means of dynamite." (Berthelot, op. cit., p. 139)

<sup>39</sup> David Keith's unusual climate change idea. Lecture 26 September 2007 as part of the TED Salon, New York. [www.ted.com](http://www.ted.com), accessed August 10, 2011.

<sup>40</sup> Keith admits that: "There's lot of mystery in the details, and there's some bad side effects, like partial destruction of the ozone layer. (...) One of the problems with sulfates is that they fall out quickly. The other problem is they're right in the ozone layer. I'd prefer them to be above the ozone layer". All the same, he believes that science and engineering evolution will find technical solutions that can overcome these disadvantages. "The one thing about this is that it gives us extraordinary leverage. These improvements of science and engineering will,

To what Utopia do we think we can still pretend? Do we support the hope of achieving a world conceived according to a depleted cultural schema, a world marked by unlimited Scientific Positivism in the service of a kind of capitalism totally dependent on energy resources totally consumed by the activities that it proposes? Should we, on the contrary, re-enchant the world (Berman 1981), inventing new ways to apprehend it, respectful of the *de facto* contract that the world and man, together with all that surrounds him and to which he belongs, have lived through together? Must not Man recognize the existence of this *de facto* contract, whether he likes it or not? From this point of view, an epistemology of chemistry, seen as a theory of knowledge, can only claim to become an object of public discussion, no longer be content to justify itself by the production of scientific knowledge and its technological applications. At the same time, the effectiveness of a systematic and reactive understanding of counter-intuitive effects of application of chemical science depends on the mobilization of many scientific disciplines. It also calls for expanded practices of deliberation, where the construction of agreements entails equally demonstration of proof (trials). For this the citizen can be considered as knowledgeable, and the scientist is to remember that he is a citizen, capable of considering, towards the same dialectic objective, himself as the other (Ricœur, 1990), and the other as another self.

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whether we like it or not, give us more and more leverage to affect the planet, to control the planet".

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# **TECHNO-SCIENTIFIC APPROACHES**

# SOME REMARKS ON THE ORIGIN, SCOPE AND EVOLUTION OF THE NOTION OF “TECHNOSCIENCE”

GILBERT HOTTOIS

## **Chemistry, A Paradigmatic Technoscience**

A major characteristic of modern science is to be physically active, creative, and productive. These features distinguish it from the ancient and traditional science that was speculative, contemplative and verbal. Now, these characteristics of modern science, which culminate in contemporary science, have been expressed in an exemplary way in the history of chemistry. It is in chemistry where we first encounter all the features that characterize contemporary technoscience: chemistry is operative, productive, creative, analytic and synthetic; it addresses the real as decomposable and recomposable in new ways, as manipulable, plastic. It also appears that it was a chemist who first has used the word "plastic" as a noun denoting an artificial substance which could be modelled at will: Baekeland, who in 1907 invented "bakelite", an early plastic. But already in the middle of the 19th century, Berthelot wrote: "La chimie crée son objet. Cette faculté créatrice, semblable à celle de l'art lui-même, la distingue essentiellement des sciences naturelles et historiques". "La synthèse, procédant en vertu d'une loi génératrice, reproduit non seulement les substances naturelles, mais aussi une infinité d'autres substances qui n'auraient jamais existé dans la nature. (...) Le domaine où la synthèse exerce sa puissance créatrice est donc en quelque sorte plus grand que celui de la nature actuellement réalisée".<sup>1</sup>

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<sup>1</sup> "Chemistry creates its object. This creative faculty, similar to the art itself, distinguishes it fundamentally from the natural and historical sciences." "The synthesis, which proceeds in virtue of a generating law, reproduces not only the natural substances, but also an infinity of other substances that never existed in nature. (...) The domain where the synthesis exercises its creative power is thus in a way larger than that of nature."

These sentences have been quoted often, but we should not trivialize their huge anticipatory scope, not only for chemistry but for our entire technoscientific civilization.

In "Challenging Standard Distinctions Between Science and Technology", Joachim Schummer, a German chemist, argues that chemistry, neglected by philosophy of science, disrupts the traditional distinctions. Chemists don't test or invent new theories; they produce new substances whose number is always growing: 95% of all known substances are artificial and are not found in nature. There were some sixteen million artificial substances in 1997 and the year before chemists had produced about one million three hundred thousand new ones. The analysis of the purposes of chemical research as they appear in scientific publications put at the bottom of the frequency scale the testing of new theories; then, in order of increasing frequency, we have: the revision of classification; the analysis of variable molecular morphology of known substances; the invention of new substances of practical use (in pharmacy, agriculture, electrical engineering, etc.). At the top of the list we have methods for improving the preparation of chemicals (new reagents, catalysts, etc.). This leads the author to the conclusion that the main aim of chemistry research is "producing new substances in order to improve abilities to produce more new substances. That is, producing new substances is actually an end in itself here—and an extremely successful one, as the exponential growth of substances demonstrates."<sup>2</sup> Showing the difficulty of distinguishing between discovery and invention in chemistry, he believes that this difference is a matter of description: we can say we discovered a new substance or reaction which leads to a law of nature; we can equally say that we invented a new substance and formalize the rules to follow in order to produce it. He concludes with a quote from Francis Bacon, which suggests that this ambiguity between discovery and invention affects modern science as such: "et quod in contemplatione instar causa est, id in operatione instar regulae est". Now, if there is one historical figure that contributed decisively to the invention of modern science as "technoscience", this figure is without any doubt Francis Bacon with his *Novum Organum* (1620) and *New Atlantis* (1627).

Today, all sciences, from particle physics to genetics, increasingly tend to create their objects, or at least tend to have an operative link with the real, not a mere cognitive relation, passively contemplative and theoretical.

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<sup>2</sup> In Lenk H. and Maring M. (Eds.). (2001). *Advances and Problems in the Philosophy of Technology*. Stuttgart: Technik und Ethik, p. 217.



Nanoscience and Nanotechnology-the "nanotechnosciences"-the NBIC<sup>3</sup>-described as "convergence"-make permeable the traditionally established epistemological and ontological borders between inert, living, thinking, natural and artificial, since they operate at the common transversal level of the molecule and the atom.

A non-metaphysical but technoscientific materialism is growing. It is operative and reflexive in the sense that the cognitive and sensitive subject is itself a subtle material operative and operable object, not ontologically foreign and requiring not a specific epistemological approach, but an ethical one.

Technoscience is a creative power that has continued to express itself through the various disciplines and technologies in the whole of which we exist now. It is therefore regrettable that we speak so frequently of "technocracy", referring to technoscience, and so rarely of "technopoiesis", which captures much better their role in creating the future. This qualification involves neither the abandonment of science and technology in favour of literature and art, nor the abandonment of the ethical review of what is created. Indeed, the relationship between an active, practical science and practical reason, that is to say moral philosophy, is obvious. A contemplative and verbal science, mirror of an essentially immutable world, did not raise such questions. It could conceive itself as pure and innocent, but it was also powerless. In the case of chemistry, the ethical questions raised are of a direct collective scope: they are economic and political.

In the late 19th century, the synthesis of dyes ruined a region of the South of France that lived thanks to the production of natural and traditional red "madder" extracted from the plant of the same name. In the 20th century, the synthesis of flavors-vanilla, cocoa, etc.-upset the economy of developing countries. Examples of this kind are legion. And with the invention of "mustard gas" (yperite), chemistry has highlighted the military use of technoscience and the specific ethical issues that such use of science raised long before the atomic bomb.

Manipulative, productive and creative, chemistry-which approaches the real as plastic-combines well with what has been called "the technological imperative": Ought Implies Can; if something is possible, it must be tried, we must actualize all the potentialities of the real. This imperative has a more or less explicit ontological postulate: anything is possible, or, at least, nothing should be considered a priori or permanently

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<sup>3</sup> Nanosciences/technologies-Biotechnologies-Information technologies-Cognitive sciences.

impossible as such. The amorality of this technological imperative has been stressed.

Indeed, to be ethical often consists in choosing freely not to do all what we could do, limiting freedom deliberately. The question arises, however: on the basis of what, in the name of what should the actualizing of the possible be limited? One answer comes from the ethics of conviction following which some things are declared sacred, inviolable, that is to say that one has no right "to touch" them. But the ethics of conviction are numerous and diverse and mankind has always been artful. An ethical attitude more in line with the positive management of the technoscientific age is the ethics of responsibility.

This last point calls for acting and intervening, but with a focus on anticipation and responsibility for consequences. This ethic is in agreement with an experimental but prudent attitude, anxious to regularly assess the implications of actions, monitoring and correcting the output, reviewing behaviour, evolving. Such an ethic is pragmatic, and pragmatism is not static or flat. Active and creative, pragmatism takes into account the complexity and relativity of the context of any enterprise. However, the ethics of responsibility makes sense only if it also gives itself a conception of the good.

This good could be the enrichment of the real, that is to say the always-growing actualization of possibilities, but under the condition of not forgetting or destroying the possibilities already completed. To preserve what is already acquired and to fulfill new possibilities, to create more and destroy less, this should be the simple maxim of an active and responsible ethics. We need museums and reservations as well as laboratories and building sites; memory is as valuable as imagination; memory is even the condition of imagination: without memory imagination quickly becomes repetitive and unsophisticated, poor.

These remarks are valid not only for activities related to chemistry; they are about our technoscientific civilization in general. Activities related to chemistry occupy in the history of the rise of this civilization and in the qualification of the epistemological and ethical site of modern and contemporary science as "technoscience" a paradigmatic place insufficiently emphasized.

It is to the largely unknown and perhaps surprising genealogy of this notion of "technoscience" that we devote the rest of this study.

## **The Philosophical and Science-fictional Original Context and Meaning of “Techno(-) Science”**

I coined the term “technoscience” in the 1970’s with both a positive and a negative aim. Positively, it was a more appropriate name for contemporary science. Negatively, it provided a basis for criticizing the traditional philosophical conception of science as fundamentally theoretical and discursive. At the same time, it denounced most of the 20<sup>th</sup> century philosophy as almost exclusively self-referential and non-referential discourse unable to face reality-the technoscientific reality-and the radically new questions raised by technoscience. This critical diagnosis applied to Anglo-Saxon linguistic philosophy, as well as to German phenomenological hermeneutics and to French structuralist, grammatological, or deconstructionist philosophy.

I introduced the concept of technoscience in order to indicate the direction in which new philosophically relevant questions could be raised, questions that would be meaningful and referential again. The first mention of “techno-science” is in my PhD thesis (T) publicly defended in 1977 and published as a book in 1979: *The Inflation of Language in Contemporary Philosophy* (L). The first sentence in which the term appears goes: “My thesis argues that what contemporary philosophy cannot or will not see is techno-science: the cosmic confrontation devoid of true light that is going on in it, the cosmos with its transhuman possibilities.”<sup>4</sup> (L, p.52).

I used also “posthuman”. But I preferred “abhuman” that I found broader, less supportive of implicit assessments. It could apply to all extraterrestrial forms of life as well as to the diversity of “descendants” of man, higher, lower or just radically different from today. “Abhuman” connoted spontaneously diversification, so characteristic of terrestrial life evolution.

Two kinds of texts inspired me: SF stories and non-narrative texts of speculative futurology. Main references were for Stanislaw Lem, Arthur C. Clarke, Fred Hoyle, Herman Kahn, Gerard Klein, Carl Sagan, Robert Jungk, and a few more. I had read a lot more (especially French SF of the 50s and 60s), but I thought that the direct philosophical interest and

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<sup>4</sup> “L’hypothèse (que défend ma thèse, GH) : le forclos (de la philosophie contemporaine) est la techno-science, l’affrontement cosmique dépourvu d’authentique lumière qui s’y pratique, le cosmos aux possibles transhumains. Est-ce par suite de la mainmise de plus en plus étendue et complexe de la technoscience sur le réel, que la philosophie a perdu la référence ontologique ?” (T, p.17; L, p. 52).

academic relevance of most of this literature was limited. Developing the concept of technoscience from SF meant for me neither to reduce SF to the expression of psychology, ideology or its criticism, nor to the pure literature offering the pleasures of intra-and inter-textuality. What interested me-and indeed still interests me-was "hard SF", or "hard speculative fiction". How did I characterize technoscience from this fictional background?

## **Technoscience and the End of Mankind**

Technoscience is closely linked to the question of the end of mankind. Not in the sense of its final aim, but its disappearance by mutation or annihilation.<sup>5</sup>

A purely anthropological conception of technoscience misses this trans-anthropological scope.

## **Technoscience and the Future**

Characterizing technoscience by reference to the future is obvious. But what I meant was the distant, very distant future, of which I tried to evoke the strangeness, the potential otherness using an analogy reversing the temporal vector. The strangeness of the far future could be as deep as the strangeness of the terrestrial forms of life hundreds of millions of years ago compared to our civilization.

The otherness of distant time, however, does not necessarily mean lack of bridges, links and therefore some continuity. But these bridges, which link us to paleontological life forms, are not defined or operated by language, through historical or logical discourse. You may narrate the process after the fact. But actually what connects us to the very distant past are not sequences of words and meanings, but genetic, chemical, physical sequences and operations: extralinguistic material links. The distant future should be evoked as radically open and opaque. My concept of "technoscience" is *not* born in the context of imagining the near future where socio-political criticism or utopianism and dystopianism prevail. It was all but the contrary.

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<sup>5</sup> "Techno-science could and should intervene in the modalities of extinction and / or mutation of the human." (L, p.303).

## **Technoscience is Operationality, Not an Issue of Language**

Technoscience is made of technical and mathematical operations, which are not reducible to discourse. Technoscience approaches human language through naturalization and machin(iz)ation.

To explore the question "What is man?" is to understand not only in the guise of hermeneutics, speculative and narrative discourse, but also in the form of techno-scientific experimentation, which is biophysically transformative and inventive. Speech, the narrative, may accompany and recapitulate, perhaps even anticipate a little. But discourse cannot replace operation and process. This marks the limits of the SF that is language. But SF points in the direction of techno-operation, which expresses the will, the desire or the fear to actually engage in it. The rich diversity of the fictional imagination helps preserving the openness of the technoscientific exploration of the future.

### **Technoscience and Ethics**

At the end of my thesis (and book), I expressed doubts about how to develop the new questions raised by technoscience and futuristic imagination: "Are they ethical issues?".

The reason for this hesitation is that the categories of ethics are "human, all too human." Moral sensitivity and conscience belong to the human form of life. Values and norms are historical and cultural. How could these categories allow us to assess and decide earnestly and freely the future of mankind, or help us make deliberate evolutionary choices?<sup>6</sup>

However, although unsatisfactory and not without risk themselves, the ethical categories seemed "the least inappropriate" (L, p. 363) if we want to address seriously all these new issues from a philosophical perspective. These issues were already starting to receive attention in the 1970s, especially through the emerging bioethics in its institutional forms (T, p.475, note 175).

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<sup>6</sup> Being an inherent part of the human form of life, is ethics not inherently inclined to put "the ultimate dignity of man" in "the acceptance of its nature (especially the limits of finitude)" definitively higher than the "boldness and the risk of transgressing its finite given nature?" (L, p.368).

## Socio-political Origin and Meaning of Technoscience

Independently, "technoscience" has been also introduced during the seventies in the USA in the context of environmental and political studies. Most important is *Governing Science and Technology* by W. Henry Lambright who talks about the "technoscience agencies" such as NIH, NASA, and so forth.<sup>7</sup> "Technoscience" refers here to "Big Science" politically organized in the wake of the Manhattan Project paradigm. But the term did not thrive. It was after the publication of *Science in Action* (1987) by Bruno Latour, that "technoscience", already widespread in France, prospered in North America. By the late 1980s, the American Society for Social Studies of Science entitled its Newsletter: *Technoscience*. A growing number of authors engaged in "science studies" or "cultural studies" started to use the term during the 1990s, such as Donna Haraway, well known by SF critics.

Overall, these approaches describe technoscience as the activity of human groups: scientists, technicians and their allies. The psychological, sociological, professional issues, economic and political aspects are highlighted. Thus described or narrated, technoscience provides no incentive for speculation or fantasy about "abhumanity". It is only "human, all too human."

What is most striking is the tendency to reduce technoscience to its political significance and subsequently to the rhetorics it employs to achieve its ends. We are in the *intertextual*.<sup>8</sup> "Science studies, cultural studies, text studies, narrative studies, etc." run into each other. Seeing technosciences exclusively not only *through* texts, *but as texts*, is a godsend for intellectuals and literary people<sup>9</sup>: it is always possible to criticize the unspoken assumptions, ideological interests, implicit values, complicities, sophistry, etc.

This evolution reverses the scope of a strongly referential neologism as well as its resistance to reductive interpretations of modern and contemporary science in exclusively or primarily social, political or even anthropological terms and in the frame of ideological criticism.

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<sup>7</sup> (1976). New York: Oxford University Press.

<sup>8</sup> Concepts of "fact," "truth," objectivity", etc. are described as purely strategic, so that one comes to think that techno-operativity is intrinsically dependent on beliefs shared by a sufficient number of people. For instance, we read in *Technoscience and Cyberculture*: "Thus, there is nothing clearly and distinctly describable as science or culture or technology." (Edited by Stanley Aronowitz, Barbara Martinsons et Michael Menster, 1996, Routledge, p. 294.)

<sup>9</sup> I mean those who have no background in hard sciences.

When this critical approach, interesting in itself, becomes unilateral, it tends to obscure what constitutes, since the beginning, the core of modern science and technology: operativity, material, technical, mathematical, extralinguistic, independent from human subjectivity and intersubjectivity, and which puts mankind into question theoretically *and physically*. After having over-emphasized the “abhuman” dimensions of technoscience-its dimensions of transcendence at once nostalgic and opposed to religion and metaphysics-the subsequent use of the term stresses too exclusively the immanence of technoscience into society and humanity as they are today and dream of the near future in a more or less utopian or dystopian continuity.

In my opinion, the best descriptions of technoscience issues are those that succeed in doing justice both to its social, political, economic, psychological, etc, immanence *and* to its operative powers to transgress the limits of the human, the naturally and culturally given. This is a potential without *a priori* limitations because technosciences only recognize empirical limits, *i.e.* contingent, existing only as long as they are not overcome.

That is why postmodern approaches of technoscience stressing hybridism and transgressing the traditional boundaries between natural/artificial, human/non human, material/symbolic, etc, are the most interesting.

From the 1990s, in my own publications as well as in my participation in bioethics committees, I tried to contemplate the human aspects of scientific issues, without losing sight of its potential for operative transgression and transcendence.

By tapping into the 1990s and after 2000, one could multiply examples of speculative theory and fiction indefinitely illustrating the concept of technoscience especially in its socio-critical uses, but also according to its scope of operative transcendence. Note that since a decade or two post-trans-humanist movements who present themselves as philosophical, scientific-technical, *i.e.* not purely fictional, are increasingly visible also in Europe, including France and Belgium.

## Conclusion

There are two extreme ways to describe technoscience.

The first emphasizes the reality of operation, technophysical, non-symbolic objectivity, and its ab-trans-post-human scope, indicating an operative, (not a symbolic) transcendence.

The second emphasizes human reality, the all too human sides of science and technology and believes that the keys of the present and all

future remain in the symbolic: discussions, debates, rhetoric, new human relations, and new institutions. Immanent to society, it does not radically question human nature defined since Aristotle as the symbolic animal, the *zoon logon echon*.

I introduced the notion “technoscience” stressing the first sense, in response to the particular historical philosophical context of the 1960s and 1970s, inspired by a number of SF readings.

Today, I still think that dropping the primitive sense completely in favor of the second betrays the concept and reality of technoscience. On the other hand, including in this concept all the human aspects without ignoring the dimensions of operative transcendence constitutes a necessary enrichment of the notion. Human technoscience transports, theoretically and practically, at the limits of human nature and reason.

It belongs to a materialistic philosophy without metaphysical definition of materialism or more simply of “matter”.



# CHEMISTRY AS A TECHNOSCIENCE?

BERNADETTE BENSAUDE-VINCENT

## Introduction

It is a common complaint that the philosophy of chemistry has been neglected in mainstream twentieth-century philosophy of science and that philosophers' views have been distorted by an undue attention to theoretical physics.

For instance Joachim Schummer used today criteria for the evaluation of scientific activity to point out a paradox: Chemistry is by far the largest scientific discipline in terms of the number of publications indexed by the major journals of abstracts. Nevertheless there are few philosophical studies of chemistry compared to other scientific disciplines. Thus, twentieth-century philosophy of science virtually ignored the major part of scientific activity. "Had those philosophers without prejudice gone into the laboratories, Schummer noticed, then they would have stumbled on chemistry almost everywhere". (Schummer, 2006, p. 21)

This reasoning was meant to emphasize the prejudices, which oriented the philosophers' attention towards theoretical issues and the subsequent increasing gap between philosophical reflection and science in action.

It is for similar purposes that the Belgian philosopher Gilbert Hottois coined the term 'technoscience' in the late 1970s. He sought to alert philosophers that by confining themselves to the analysis of language and logic they were blind to the dramatic changes going on in the world around them. (Hottois, 1984) The term technoscience was meant to emphasize not only that technological applications were a prime mover of scientific research but also that a lot of technology is embedded in science. (Hottois, 2006)

The similarities between the two polemical charges against "the linguistic turn" in twentieth-century philosophy of science invite to look further at the rapprochement between chemistry and technoscience. *To what extent the identity of chemistry could be reconfigured as a technoscience?*

Obviously the answer to this question requires a precise definition of the rather loose concept of technoscience. However there is nothing like a standard and consensual definition of this term, which could be referred to and be confronted to a standard definition of chemistry. I will consequently refer to different definitions of technoscience—from the weaker to stronger notions. Finally I will argue that the problem has to be turned inside-out and is better addressed as: *To what extent the emergence and fashionable uses of the notion of technoscience over the past three decades did change the identity and the status of chemistry.* In other terms, the concept of technoscience will help me to emphasize the changes occurred both in the philosophical perspectives on chemistry, and in the practices of chemistry.

This attempt relies on a presupposition that should be clarified from the outset: that there is no fixed, transhistoric identity of chemistry. The view of chemistry as a historical construction, continuously reconfigured by the contexts of its practices, is one major result of the *History of Chemistry* that I co-authored with Isabelle Stengers.

## **Technoscience as Interaction of Science and Technology**

In 2005 two issues of the journal *Perspectives on Science* applied the concept of technoscience to chemistry in a discussion of the “technoscientific productivity” of experimental sciences. For instance Ursula Klein argued that 17<sup>th</sup> and 18<sup>th</sup> century chemical research was technoscientific *avant la lettre*. (Klein, 2005b) And Hans-Jörg Rheinberger claimed that the notion of “phénoménotechnique” that Gaston Bachelard forged to characterize 20<sup>th</sup> century physics and chemistry was a precursor of technoscience. (Rheinberger, 2005) The inclusion of chemistry in the extension of the concept of technoscience was based on the following definition of technoscience as “firstly, the alliance of modern science, technology and industry; and, secondly, the technical shaping and production of scientific objects within the experimental sciences”. (Klein 2005, p. 139) In this view chemistry is a technoscience for two major reasons: because of its dual face as science and technology and because there is a lot of techniques embedded in experimental practices. This perspective interestingly broadens the scope of the history and the philosophy of chemistry.

From a historical perspective, the emphasis on technological aspects prompted a deep revision of eighteenth century chemistry. In the early twentieth century historians of chemistry evaluated the advances in chemistry from the standpoint of the standards and values of physics. In the standard view, the emergence of modern chemistry was described as

the result of the adoption by chemists of atomic and mechanical theories. Hélène Metzger for instance argued that alchemy was defeated by Cartesian corpuscularism. (Cardwell, 1968; Siegfried, 2002) Most historians of chemistry considered alternative theories based on qualitative principles and elements as « errors » that had to be overcome. In paying attention to laboratory procedures historians of early modern chemistry such as Lawrence Principe, and William Newmann gave an alternative account of the transition between alchemy and modern chemistry: not only many principles and practices characteristic of modern chemistry were already familiar to alchemists but also “chymists” had a way of their own to get out of the scholastic paradigm and embrace experimental philosophy. (Newmann & Principe, 2002)

The historiography of the chemical revolution centred on Lavoisier’s theoretical achievements by Henry Guerlac (1961) and his followers was divorced from the study of the chemical revolution that occurred in technological modes of production as described by Clow and Clow (1952). So different were the stories told by historians of science and historians of technology that one could believe that there were two radically different cultures of chemistry in the eighteenth-century.

This view has been radically changed by historians of chemistry such as Larry Holmes who reacted against the privilege of matter theories and emphasized the role of the laboratory practices.

The problems and objects of study of chemistry have been provided by and limited by the operations that could be performed on materials in a chemical laboratory [...]. As theoretical structures changed and new objectives supplemented or displaced older ones, the stable setting of the chemical laboratory both identified chemists and distinguished them from other natural philosophers who dealt with some of the same phenomena that concerned them. (Holmes, 1993, p. 478)

Taking seriously the painstaking laboratory work, which conditions the production of chemical knowledge, Holmes developed new perspectives on eighteenth-century chemistry. (Holmes, 1989) No longer was it centred on phlogiston theory—its triumph and defeat by Lavoisier. It was a flourishing experimental science with a collective investigative pathway and a conceptual framework of its own. More recent historical studies on the pedagogical practices of chemistry in the eighteenth-century confirm the intricacy of academic culture and craftsmen practices.

The philosophy of chemistry benefited from historiographical revisions. Historians of chemistry are venturing new philosophical perspectives. For instance Ursula Klein and Wolfgang Lefevre *Materials in Eighteenth-*

*Century Science: A Historical Ontology*, bridges the gulf between the history of chemical science and the history of chemical technology by focusing on materials rather than on heroic figures. (Klein & Lefevre, 2007) Materials are rightly defined as ‘boundary objects’ connecting academic science and craftsmen cultures. The authors remind us that laboratory science produces artefacts. They remarkably emphasize that 18th century chemistry belonged to “experimental history”, and developed techniques for identifying and tracing material individuals, or “pure substances”, out of necessity for daily practices.

The shift from the linguistic turn to the practical turn has hardly begun in the philosophy of chemistry. Only recently philosophers did timidly broaden the scope of the philosophy of chemistry beyond the traditional issues of the theoretical foundations of chemistry in quantum theory and reductionism. In the collective volume published in 2006 by Davis Baird, Eric Scerri and Lee McIntyre only one third of the volume deals with the traditional issues. The attention has shifted to actual practices displayed by chemists: such as computer-aided process design, molecular imaging and electron microscopes. The appropriation of physical instruments by 20<sup>th</sup> century chemists and promotion of their own instrumental culture sheds a light on the chemical ways of measuring and theorizing. (Reinhardt, 2006) It is important in my view to further broaden the scope of the philosophical studies of chemistry and to expand it to industrial or agricultural practices of chemistry. So chemistry can be approached as a technoscience if the internalization of technology in its investigative practices and its dual face as pure and applied science are fully taken into account.

## **Technoscience as Impure Science: A Polemical Notion**

Nevertheless technoscience is not just a mixture in various proportions of two ingredients, science and technology. Just as a mixt is something different from the sum of its components, technoscience is something different from both science and technology. “Technoscience” is an alternative to “science and technology” with its assumption of two distinct but interacting spheres. ‘Technoscience’ is not a neutral descriptive term. It is not a disciplinary label that would refer to a subset of the sciences.

Bruno Latour used the term in *Science in action* as shorthand for a fusion of “science-and-technology,” that is, as a hybrid where the two cannot be separated out from one another in terms of basic and applied research. (Latour, 1987) For Latour and in a rather different way for Donna Haraway, (1997) the concept of technoscience points to the true

face of science once the complex alliances between human and non-human actors, nature and society are acknowledged. The notion applies to the construction of scientific objects as well as technological objects by a multitude of heterogeneous actors “no matter how dirty, unexpected or foreign they seem”. (Latour, 1987, p. 174) This concept is meant to deconstruct the purified image of science, as a purely cognitive, autonomous, disinterested, enterprise.

With its polemical connotation, the notion of technoscience proved useful to describe chemistry as an “impure science”. (Bensaude Vincent & Simon, 2009) The philosophical interest of chemistry is based precisely on the fact that it resisted the process of purification of science. It is impure not just in the sense that it pollutes air, contaminates soils and poisons rivers. It is impure because it challenges the purified image of science that prevailed in the 20<sup>th</sup> century. Its epistemological specificity and its ontology are closely associated to its “impurity”. The ontology of chemical substances, in our view, springs from the chemists’ activity of transformation of matter rather than from the inner structure of the atoms lying behind the phenomenological materials.

The epistemology of chemistry can be adequately defined by the phrase “knowing through making”. Laboratory chemical practices are not just aimed at testing preconceptions or theoretical hypotheses. Chemists do not use the mediation of instruments to understand natural phenomena, like experimental physicists do. The laboratory determines the object of chemical investigation. Chemists have always used the detour of the laboratory to access nature. Only man-made, artificial products provide information about natural substances. As the etymology of the term (coined by chemists) reminds us, the laboratory is a place of labour, of manual work rather than of inductive or deductive reasoning. The knowledge of nature can be obtained only at the cost of painstaking experiments, as Van Helmont used to claim. (Newman & Principe, 2002, p.180) Despite the importance of chemical theory for experimenting, chemistry is first and foremost concerned with making.

As making is the chemists’ highly praised activity and the major part of the work found in academic publications, chemists have a distinctive way approach to laboratory experiments. It is both a material practice and an intellectual practice. Theories are rarely meant at explaining phenomena by deriving them from a general law or from quantum physics. This deductive type of explanation is what Roald Hoffmann calls a “vertical explanation” and he argues that these explanations convey no chemical understanding of phenomena. (Hoffmann, 2012) Chemical theories are more like narratives, telling the story of what is supposedly

going on in the black box of the flask where a series of reactions take place. Unlike physicists chemists are not primarily interested in clarity and distinctness, and do not hold consistency to be a very high value. They don't rely exclusively on epistemic criteria for accepting a theory. Just as early modern hooked and spiny atoms were a "Cartesian novel", modern electronic orbitals could be regarded as a "quantum novel". Rather than being ideal accurate representations of nature, theoretical narratives display meanings, with atoms and molecules best described as actors in a story. Even when these invisible entities are visualized using imaging techniques, they do not mirror the ultimate reality underlying phenomenological appearances, although they do *mean* something for the chemists. In certain cases they may mean that there is a possibility of breaking a bond, or of substituting a functional group or of encapsulating certain atoms within a cage molecule, etc. In addition stories require a temporal structure: temporality plays a prominent role in chemical narratives as the kinetics determines whether the reaction will be a success story or not.

The ontology of chemistry should be re-examined accordingly. The traditional realism/positivism debate is not adequate to chemistry. Rather than framing the debate in terms of the question 'what can one know?' it might be better to pose the question 'what can one do?' and then examine the ontological consequences. I suggest the term "operational realism" to emphasize that chemists do not claim to represent the real structure of material substances. They rather aim at identifying specific dispositions for operations. They are interested in capacities and believe in the reality of their agencies. Operational realism is akin to Hacking's "entity realism" but should be extended to abstract concepts such as elements as well as concrete entities.

So chemistry can be redefined as a technoscience in the Latourian sense of the term as a science that is indifferent to the ideal of purification that defines "science" in the singular.

## **Technoscience as an Ideal Type**

It is not sufficient however to present chemistry as an alternative to the ideal type of pure science. Technoscience is not just a polemical notion used by social scientists to deconstruct the mythical image of science; it has become a model in itself. The historian of science Paul Forman defines technoscience as a reversal of the values attached to science. (Forman, 2007) Whereas modernity was characterized by the high cultural rank of science and scientists—"the primacy of science to and for technology" —,

post-modernity, according to Forman, is characterized by the primacy of technology over science. And he argues that this inversion occurred in the 1980s and was encouraged by social studies of science.

Without endorsing Forman's view of an epoch-making transmutation of values, his perspective is interesting because it provides an additional distinctive feature to the definition of technoscience. The notion of technoscience denotes not only the actual hybridization of science, technology, commercial and industrial interests but also a new ideal of scientific practice where epistemic values (such as truth, simplicity, etc.) are explicitly challenged by non-epistemic values such as social robustness, social and economic relevance, and sensibility to environment.

As approximations of this new ideal-type of value-laden sciences, one can think of Materials Science and Engineering, of genomics or nanotechnology. These recent research fields are all hybrids of science and technology. More interestingly they are actively promoted by science policy makers with the expectation that they will bring about potential solutions to all kinds of societal, environmental and economic problems. Far from being neutral they are presented as serving certain values such as durability, human enhancement or solidarity.

In stark contrast to the purification of scientific research that prevailed in the mid 20<sup>th</sup> century, these emerging fields are repeating the "economy of promises" developed by medieval alchemists who claimed to be able to provide immortal life or by modern synthetic chemists who claimed to bring food, health and welfare all over the world. More broadly a distinctive feature of chemistry is that making molecules is presented as a means towards an end: it can be healing or killing, bringing health or death, or creating a beautiful architecture. In any case, chemistry is loaded with values such as public good, utility, beauty. In this respect the emerging technoscientific research fields are mimicking chemistry more than physics.

In the convergence of disciplines chemistry may be seen as a model science for renewing biology. Synthetic biology, an emerging discipline aimed at engineering living organisms can be seen as a modern replica of nineteenth-century synthetic chemistry. Molecular biology and genome sequencing would thus be considered as a kind of analytical biology that paved the way for the emergence of synthetic biology. (Yeh & Lim, 2007; Bensaude Vincent, 2009) In their attempt to move beyond the limits of descriptive biological science, synthetic biologists have adopted the epistemological style of chemists: they express their credo in knowing through making through repeated quotations of Richard Feynman's alleged words "What I cannot create I do not understand".

## Challenged Disciplinary Identity

Transdisciplinarity is a major feature of recent technosciences such as nanotechnology and biotechnology that could differentiate them from the chemistry. However, today most chemists are also working beyond the borders of their niche. Many of them are practising chemistry in multidisciplinary groups and they play a crucial role in materials and nanotechnology research. What can be the impact of such multidisciplinary collaborations on the identity of chemistry? Does it make sense to develop the project of a philosophy of chemistry as a discipline when disciplinary boundaries are more and more blurred in the actual practices of chemists?

Through their collaborations with other specialists in multidisciplinary projects chemists have significantly changed their practices; in particular their *linguistic practices*. The term “material” has become fashionable and displaced the more traditional term “substance”. Similarly the phrase “molecular machine”, popularized by the pioneers of nanotechnology, is now appropriated by chemists who rather used to think of themselves as creating “molecular “molecular architectures”. For instance the exotic architectures of the catenanes and rotaxanes are now described as nanomachines. Such vocabulary shifts may be the symptoms of more radical philosophical changes.

In adopting an engineering view of nature, chemists less and less consider the periodic table as a foundational system and tend to look at it as a practical toolbox, a kind of department store where to find materials or devices. One could say that the periodic system charts ‘affordances’ rather than simple ‘dispositions’ because the elements arranged in the system blur the dichotomy between the subjective and the objective, while being real, and material. (Harré, 2003) For instance the dispositions of carbon molecules with their robust and stable structures are actualized in the DNA backbone. The large potential of combinations of carbon atoms afforded the incredible variety of synthetic compounds. Carbon also affords the hollow space of nanotubes as well as the thin monolayers of graphene. It is seen as an endless source of functional properties that can only be visualized, performed and instantiated by the combination of material dispositions and intentional contrivance.

However this reconfiguration of chemical elements as affordances does not really threaten the disciplinary identity of chemistry. On the contrary, the mixt of disciplinary identities in current research programs seems to revitalize the pride of chemists. Up to now, the disciplinary identity of the chemical community proves extremely resilient. Chemists engaged in Materials Science or nanotechnology clearly express a feeling of



belonging to the chemical tribe. On the occasion of an interview a member of the Materials Research Society nicely used a chemical metaphor to express his attachment to the chemical tribe: He compared the bonds that attached him to Materials Science and Engineering to weak van der Waals forces while he argued that he was still linked to chemistry by strong covalent bonds.

Unexpectedly materials research, biotechnology and nanotechnology are reviving the great ambitions of 19<sup>th</sup> century chemists of penetrating the secret of life. For instance leading figures of chemistry such George Whitesides and Jean-Marie Lehn deliberately drop the positivistic attitude of prudence that is often considered as typical of chemists. They do not hesitate to address big metaphysical questions. Far from confining their work to the production of useful materials, they want to expand their area of competence to questions such as the origin of life and even the origin of consciousness. Whitesides claims that chemistry is everywhere and must go everywhere. By using all kinds of chemical bonds, chemists are expanding the territory of chemistry and they are in a position to decipher the most complex phenomena of life and even cognition: "The nature of the cells, he claims, is an entirely molecular problem. It has nothing to do with biology". (Ball, 2006, p. 501)

Similarly as Lehn moved from supramolecular chemistry to Constitutional Dynamical Chemistry he revives the greatest ambitions for chemistry. He portrays chemistry as the "science of informed matter", a core science mediating inanimate matter (materials process) and animate matter (living organisms and their complex behaviors). (Lehn, 2006)

## Conclusion

The philosophy of chemistry can no longer ignore that chemistry is a technoscience at least if this concept is given all the spectrum of meanings acquired over the past decades. Those who stick to the weak meaning of technoscience-as the close interaction of science and technology-will describe chemistry as an exemplar "phenomenotechnique" and as a model utilitarian science. Those who are more inclined to adopt the Latourian demystifying meaning of technoscience, will describe chemistry as an impure science, challenging the canons and moral economy of the ideal of pure science, which has attracted the attention of philosophers for too long. Describing chemistry as an impure science is in fact denouncing the irrelevance of mainstream philosophy of science since World War II. They will call for a profound re-thinking of the curriculum of philosophy of science courses around the world.

Finally those who tend to consider technoscience as an alternative ideal promoting value-laden, project-targeted, and cross-disciplinary research will come up with an additional problem to address. Yes chemistry will help reform the entire field of the philosophy of science because it is closer to the new ideal-type of knowledge society than many other disciplines. Most of its characteristic features such as “knowing through making”, the emphasis on “operations”, and the “ontological indifference”<sup>1</sup> seem to permeate through a variety of research fields. The relevance of a disciplinary approach of the philosophy of science should no longer be taken for granted: it becomes an issue in itself. How are we to understand the chemists’ claim for a strong disciplinary identity for their strong attachment to their ideal of disciplinary identity?

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<sup>1</sup> This phrase is used by Peter Galison to characterize technoscience. Galison, “The pyramid and the ring. Presentation at the conference of the Gesellschaft für Analytische Philosophie” (GAP), Berlin, 2006.

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# MATERIALITY AND ABSTRACTION IN MODERN CHEMISTRY

URSULA KLEIN

It has often been stated that modern chemistry is marked by a shift away from impure and useful materials towards pure chemical substances. Antoine-Laurent Lavoisier has been identified as a key figure in this historical process. Accordingly, his self-proclaimed chemical revolution has been described as a rupture in chemists' study of material substances, which privileged chemical analysis, purity and detachment from technological uses of material substances.<sup>1</sup> Simultaneously, so the story goes on, chemistry was cleaned from its pharmaceutical and artisanal heritage and thus transformed into a "philosophical chemistry" or pure science.<sup>2</sup> Predominant or exclusive concern with pure substances thus becomes the hallmark of pure science. The following is a critique of this view along with a presentation of an alternative picture of early modern chemistry.

## **Abstract Concepts Versus Chemists' Practice**

The argument that modern chemists have always studied pure chemical substances independent of the substances' useful functions is questionable from several perspectives. From a philosophical perspective the argument conflates abstract concepts with chemical practice. From a historical perspective it ignores changes of meaning of the concept in history. If we historicize the concept of purity we see that it even converged with usefulness in former times, namely in the tradition of Paracelsian alchemy (see below). Furthermore, Lavoisier and his collaborators neither introduced a new concept of pure chemical substance nor deeply changed chemists' laboratory practice with material substances. As Wolfgang Lefèvre and I have demonstrated in our *Materials in Eighteenth-Century*

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<sup>1</sup> See, for example, Bensaude-Vincent, *Lavoisier*.

<sup>2</sup> See Kim, *Affinity*.

*Science*, the concept of pure chemical substance involved in the *Méthode de nomenclature chimique* (1787) by Lavoisier and his collaborators and the concept of chemical purity presented in the eighteenth-century tables of affinity (since 1718) were the same concept.<sup>3</sup>

In eighteenth-century chemistry the term “pure” substance meant a single kind of chemical substance, as distinguished from an apparently homogeneous mechanical mixture of different kinds of substance. “Impure” substances were defined as particular cases of mechanical mixtures; a substance was impure when small quantities of additional kinds of substances were mechanically mixed with it. This concept of chemical purity was closely related to the modern concept of chemical compound.<sup>4</sup> It is present in both the eighteenth-century tables of chemical affinity and in the *Méthode*. The symbolic mode of representation used in the eighteenth-century tables of affinity allows to grasp this meaning at a glance: one symbol of the affinity table denoted one kind of pure chemical substance. Furthermore tables of affinity highlighted a criterion for the modern notion of pure chemical compound that was taken for granted and thus tacitly presupposed in the *Méthode*: affinity. It was affinity that demarcated a pure chemical compound from apparently homogeneous mechanical mixtures. Putting it in Alan Chalmers’s words, affinity tables manifested that “components of a compound are indeed combined by virtue of the rapport acting between them and it is this combination via a rapport that distinguishes a compound from a mere mixture.”<sup>5</sup>

### Abstraction

The concept of pure chemical compound involved in the eighteenth-century tables of affinity and the *Méthode* presupposed abstraction. Many sensible properties of substances (such as color, smell, taste and consistency), their natural origin, and techniques of processing or production as well as practical uses were ignored.<sup>6</sup> The concept abstracted

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<sup>3</sup> See Klein and Lefèvre, *Materials*.

<sup>4</sup> For a more detailed argument see Klein, *Material Substances*.

<sup>5</sup> Chalmers, *Concept of Chemical Compound*, 38.

<sup>6</sup> However, chemists did not abstract from all types of observable properties in this context. Their identification of distinct kinds of pure chemical substances did not exclusively rely on composition. First, in the case of simple substances that could not be decomposed (later: “chemical elements”) composition was excluded as a criterion for identification. Hence chemists also used as criteria for identification so-called “chemical properties,” tested with reagents, measurable, physical properties and some other observable properties (such as shape of crystals).

further from local varieties of samples of the same kind of chemical substance; local varieties were understood as effects of impurities (small quantities of additional kinds of substances mixed with the predominant one) that were insignificant for the identification of the chemical kind at stake. Thus the concept presented the *kinds* of chemical substances as if they could be directly observed in nature. It obliterated varieties as well as the social and technological context of chemists' substances, the ways in which they had access to them and the roles these substances played on the marketplace, in the household, workshop and so on.<sup>7</sup> With respect to abstraction, the eighteenth-century concept of pure kinds of chemical substances is fully comparable to the later concept of pure chemical kinds that was based on stoichiometry and represented by chemical formulas. A chemical formula represents a kind of chemical substance in an utterly abstract fashion, based on knowledge of composition, supplemented by knowledge of reactions and molecular structure.

Abstraction is involved in any concept formation, and it is a purely mental activity. This sounds trivial, but it is perhaps helpful to remind us of this fact. Abstraction concerns thinking, concept formation and naming but not practical doing with hands, instruments and material objects. Studies of abstract concepts tell us little about chemists' experimental and technological practice. Furthermore, the fact that chemists constructed concepts that abstracted from usefulness does not imply that they eschewed considerations about usefulness. Abstraction is logically different from contrariety. The eighteenth-century chemical concept of purity and the modern concept of stoichiometric purity do not mean the opposite of usefulness but rather black-box it. But more important is another issue: how did chemists' abstract thinking, representation, and naming relate to their practice and material culture? To be brief, how can we re-introduce and reconstruct the social and technological context from which the early modern and modern chemists abstracted in certain parts of their work? If we supplement studies of concepts and nomenclature with historical reconstructions of chemists' practices and the material objects involved in them, we arrive at a new picture. We then see it was not chemists' *general* goal to reduce a particular kind of material substance to a thin, abstract version of itself. The community of chemists has always been interested in substances in many different ways, depending on contexts of inquiry. While a late nineteenth-century chemistry professor teaching structural chemistry may have highlighted abstract compounds

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Identification relied to some extent on connoisseurship, since there was no general rule which observable property of a substance counted for its identification.

<sup>7</sup> See Klein, *Verbindung und Affinität*.

represented by formulas, a chemist cooperating with the synthetic dye industry took many additional dimensions of substances into account.<sup>8</sup> Moreover, chemists have studied both impure and pure substances in the long history of chemistry, and both types of substances have been applied as useful materials.

## Practice

As I have shown elsewhere in greater detail, all of the chemical substances, with one exception (i.e. “principe huileuse” or phlogiston), represented and ordered in E. F. Geoffroy’s famous table of chemical *rappports* (1718) actually were materials known and handled in mundane practices. Most of them were produced in seventeenth-century mining and metallurgy and in pharmaceutical shops.<sup>9</sup> The metals known in the eighteenth century, and ordered in Geoffroy’s table, were useful materials produced from natural mixtures (i.e. ores). Likewise the metal alloys, earths, alkalis, and acids represented in this table, were not substances found in nature, but processed natural materials used and sold as commodities. The classes of pure chemical substances grouped together in the table of chemical nomenclature published by Lavoisier and his collaborators overlapped to a large extent with the substances enlisted in Geoffroy’s table of chemical *rappports* and the subsequent affinity tables.<sup>10</sup> It thus hinged as well on the world of production and commerce. Not only the academic chemical laboratory but the artisanal laboratory and workshop too engendered pure substances—relatively pure substances, of course, depending on the instruments and analytical techniques of a given period.

In their laboratories the eighteenth-century chemists analyzed commercial and natural raw materials, and they further experimented with the isolated components of these materials. Studying the chemical reactions of the isolated components they created a plethora of new reaction products. Chemistry has been the most productive laboratory science in history. Today, millions of substances are registered in chemists’ databases. The vast majority of the present chemical substances are products of chemical research, and a significant part of these research products stem from chemical synthesis. But chemists have produced new kinds of substances not only by chemical synthesis. Their chemical analysis and studies of

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<sup>8</sup> In Klein and Lefèvre, *Materials*, we have introduced the concept of multidimensional objects of inquiry.

<sup>9</sup> Klein, *Verbindung und Affinität*; Klein and Lefèvre, *Materials*.

<sup>10</sup> *Ibid.*, 81-192.



other types of chemical reactions have been materially productive as well.<sup>11</sup> In classical chemistry, chemical analysis was performed by letting the substance A that was analyzed interact with another substance B and thereby decompose into several new substances C, D, E and so on. This kind of chemical anatomy, as it was sometimes called, differed from mathematical and physical analysis in an important way. It actually took apart substances, thereby producing new, perceptible substances, which chemists isolated and identified in subsequent experiments. The immediate result of the analysis thus was not data, diagrams, or other forms of inscriptions on paper, but material substances. Performing analysis, synthesis and other kinds of chemical reactions chemists have continually extended the world of material substances.

In the eighteenth century many of the new substances created in chemists' laboratory were pharmaceutically applied. Likewise, in the nineteenth and twentieth centuries, an impressive number of the newly prepared pure chemical substances were transferred to social and industrial sites. Think of alkaloids such as morphine, strychnine and caffeine, separated from plants and identified in the early nineteenth century.<sup>12</sup> Nineteenth-century chemists had both epistemic and commercial interests in these pure organic substances. The German apothecary-chemist Heinrich Emanuel Merck, founder of the pharmaceutical concern Merck in the 1820s, even first produced his alkaloids for trade in a quite traditional, small laboratory belonging to his apothecary's shop.<sup>13</sup> Think of the pure carbon compounds represented by structural formulas in the 1860s; these substances challenged chemists' theories and at the same time several of them became unexpectedly applied in the new synthetic dye industry.<sup>14</sup> Or think about the element radium separated and purified by Marie and Pierre Curie in 1898 from tons of pitchblende. Shortly afterwards, chemical companies started to produce radium, and a radium market developed that offered radium as a commodity to be used in luminous watches, women's creams, toothpastes, cigarettes, drinks, condoms and various medical products.<sup>15</sup>

It would lead us too far to discuss in detail the many ways in which modern chemists paid attention to useful functions of their own "chemical

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<sup>11</sup> I have published elsewhere in detail on the material productivity of classical chemical inquiry; see, for example, Klein, *Technoscience*.

<sup>12</sup> See Tomic, *Aux origines de la chimie organique*.

<sup>13</sup> Löw, Merck; Klein, *Apothecary's Shops, Laboratories*.

<sup>14</sup> Reinhardt and Travis, *Modern Chemical Industry*; Pickering, *Decentring Sociology*.

<sup>15</sup> Rentetzi, *Trafficking Materials*; Ceranski, *Tauschwirtschaft*.

substances,” created in their laboratories, and further explored their technological application as useful materials. In the highly differentiated, industrial societies of the twentieth century their institutions and methods certainly differed from those in the eighteenth century. Furthermore there is also no question that the majority of the hundred thousands of new organic compounds that have been prepared in organic chemistry since the mid nineteenth century were never practically applied. But this does not affect my principle arguments. First, that chemists’ experiments with material substances have relied on supply with raw materials, processed substances and instruments by socio-technological institutions outside the scientific world. Second, that chemistry is materially productive and continually creates new material substances. Third, that the substances created in the laboratory are not mere phenomena or experimental traces of knowledge production but also things. “Things” implies that they are also part of the physical world and have also a life of their own. They can be transferred out of the epistemological context of representation and knowledge production and into the mundane social and technological world, in which they can have many unforeseen effects. They also interact with physical bodies in intended and unintended ways.

### Epistemological Determinism

In a recent essay, which includes a critique of our *Materials in Eighteenth-Century Science*, Bernadette Bensaude-Vincent blames us that we did not pay enough attention to chemists’ abstract thinking and concept formation. She concedes that many of the eighteenth-century chemists’ substances came from the arts and crafts and that it “is appropriate to emphasize the role of craftsmen in early modern chemistry.” But then she states that our approach “nevertheless overlooks the continuous efforts to gain objective knowledge of the composition of those substances and to detach them not only from their natural origin but from their technological uses as well.”<sup>16</sup> She adds that Lavoisier’s reform of chemical nomenclature was the outcome of long-term efforts to gain objective knowledge of the composition of substances, and further repeats her argument, already presented in her book on Lavoisier from 1993, that the reform of chemical language in 1787 “banned denominations referring to local geographical

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<sup>16</sup> Bensaude-Vincent, *The Concept of Materials*, 110. It should be noted that the following remarks on Bensaude-Vincent’s approach refer to this recent paper from 2011 and to several of her older publications. In other papers, including her paper in this volume, her approach and arguments may be different.

origins or medical uses of substances in favor of denominations mirroring their intrinsic compositions.”<sup>17</sup> While the latter statement is true—and has been part of our argument, based on a detailed analysis of the *Méthode* and its table of nomenclature—it would be wrong to conclude that chemical language and practice were two sites of the very same coin and that Lavoisier’s reform of language implied a change of the entire chemistry. In her paper *The concept of Materials* (2011), Bensaude-Vincent exactly draws the latter conclusion. Thus her argument culminates in the statement, referring to Gaston Bachelard, that “the notion of materials being linked to concrete, sensory qualities, and to human interests can be considered as a typical epistemological obstacle that modern science had to overcome (Bachelard 1938).”<sup>18</sup> This statement hardly applies to modern chemists’ laboratory practice. When I studied chemistry, one of the first instructions I got in the laboratory was how to test the smell of a substance. Observation of smell, like many other sensible properties of substances, is still involved in the first identification of substances in modern chemical laboratories. Likewise, “human interests” or considerations about usefulness do have a place in modern chemistry. Think about “technological chemistry”, for example. Is modern technological or engineering science not a “science” (in the broad French sense)? To give

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<sup>17</sup> Ibid., 111. It should be noted that Bensaude-Vincent presents two, rather different arguments about continuity in eighteenth-century chemistry. On the one hand, she now acknowledges that Lavoisier’s approach was a culminating point in a long tradition; by contrast, she argued in 1993 that the new nomenclature was a true revolution, a “rupture brutale avec le passé” (Bensaude-Vincent, *Lavoisier*, 233). On the other hand, the latter argument is still reinforced today by the following statement: “Thus modern chemistry developed a specific way of dealing with individual substances that transcends their singularities in making them samples of pure chemical species” (Bensaude-Vincent, *The Concept of Materials*, 111). Bensaude-Vincent argues here that pre-Lavoisierian chemists treated substances as singularities (or “individual substances”) and that it was Lavoisier who introduced the concept of a chemical kind or species based on knowledge of composition. Thus she also states: “With the new nomenclature individual substances became commensurable samples of chemically composed matter” (ibid.); and further that nineteenth-century synthesis only “reinforced the conceptual shift from singularities to peculiarities” (ibid.). It is strange that Bensaude-Vincent denies here that the tables of affinity and certain pre-Lavoisierian chemical theories (such as the theory of salts, the theory of combustion and calcination) represented kinds or species of substances, based on the concept of chemical compound and knowledge of composition (see my argument below). If this assumption were correct, Lavoisier’s chemistry would indeed be a revolutionary rupture.

<sup>18</sup> Ibid., 110.

an example of modern technoscience, in materials science human interests do play a role, as Bensaude-Vincent is certainly aware of.

While the *concept* of pure substance and the new *names* introduced in the *Méthode* were indeed far going abstractions, the material referents, the things denoted by the Lavoisierian nomenclature, were not abstractions. Practice and materiality are concrete. The material substances denoted hydrogen, zinc oxide, sulfuric acid, oxygenated muratic acid in the *Méthode* were as much things of the material culture of the laboratory and beyond as gunpowder, Prussian blue, aromatic vegetable oils, and opium, which were impure substances and commodities identified not least by their sensible qualities. They were as explosive, colored, smelly and poisonous as the latter impure materials. Moreover, Lavoisier and many post-Lavoisierian chemists continued to take the usefulness of substances into consideration.

As we have argued in *Materials in Eighteenth-Century Science*, the new chemical language introduced in the *Méthode* must not be taken as a turning point in chemistry *tout court*. Apart from the fact that the new language did not extend to plant and animal chemistry, language did not *determine* chemists' experiments and technological activities. It affected practice, conditioned practice, but there was no one to one match between concepts or language and practice, experimental and technological. By contrast, Bensaude-Vincent's approach bans considerations about the *partial* independence of material objects from language, concepts and the boundaries of a scientific discipline. In a nutshell, I would call this approach "epistemological determinism"—the belief that material things created and involved in experiments are fully determined by their epistemic context. As a consequence, epistemological determinism reduces philosophical and historical studies of experimentally created material objects—or "experimental phenomena," as they are often called in that epistemological framework—on the study of their place in the generation of knowledge. It obliterates modern chemists' concern with the usefulness of their substances, and it ignores the existence of modern technological chemistry and chemical engineering alongside university-based chemical science. Hence it is just the acquisition of objective knowledge that interests Bensaude-Vincent and not the material products of classical chemical analysis, the unintended effects of chemically prepared substances, and the unforeseen applications of newly prepared material substances outside of the laboratory. The latter themes do not fit a research agenda under the auspices of epistemological determinism.

In the laboratory Lavoisierian and post-Lavoisierian chemists could not abstract from the sensible properties and physiological effects of the

substances they worked with. Nor could they abstract from their natural and commercial origins. On the contrary, it was of great interest to them whether the apothecary or merchant who sold them materials was reliable or prone to fraud. Adulteration of materials in trade was a permanent concern of eighteenth-century and early nineteenth-century chemists. It was as important for them as the question of whether they had reliable instruments to analyze and prepare substances. Furthermore, as a matter of fact in the long history of chemistry chemists have rarely been disinterested in possible applications of a newly prepared substance. While social institutions and methods that fostered the transformation of a newly prepared laboratory substance into a prototype of a useful material changed in the history of modern chemistry, the principle constellation did not change: any material substance produced in the chemical laboratory has the potential to be applied outside of the laboratory in technology and society.

Unlike social entities, material things have also an existence independent of us. Once brought into being, they can exist independent of our knowledge and talk about them. Generally speaking, in classical chemistry chemical substances can even exist independent of the chemical apparatus that chemists used for their creation. They can be taken out of the original test tube in which they were prepared and transferred to another laboratory vessel. Samples of a newly prepared substance can further be transported outside the scientific laboratory to be examined and reproduced, for example, in the laboratory of a chemical engineer or industrialist. There are many possibilities to use a material substance independent of the original goals and interests of its producer. And these possibilities are, in principle, open-ended. It is well known that instruments can be used for goals their inventors never dreamt of, and so can substances. For example, hydrogen and oxygenated muriatic acid (chlorine), isolated and clearly identified (or “discovered”) in the 1760s and 1770s, were used in contexts outside chemistry before the end of the eighteenth century.<sup>19</sup>

New uses often come with the discovery of new, unexpected properties and effects of a material substance. Novelty emerging from the surplus of materiality over knowledge can be seen as an advantage or disadvantage. Thus material objects have been described as generators of exciting surprises.<sup>20</sup> Alternatively, one might deplore unintended side-effects and loss of control. Historians of science and technology have long discussed

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<sup>19</sup> Hydrogen was used for ballooning and chlorine for the bleaching of textiles.

<sup>20</sup> See Andrew Pickering in this volume and his other work.

issues relating to the themes of loss of control and unintended consequences of our doing. It is time for a systematic discussion of these themes in the philosophy of science. As material things, chemists' substances, impure and pure, have the potential to act in unforeseen ways and to be practically used outside the chemical laboratory. The substances created in the laboratory are not determined by chemists' epistemic goals. To use a well-known phrase of Ian Hacking, laboratory substances can have a life of their own.<sup>21</sup>

### **Usefulness of Objective Knowledge about Chemical Composition**

Bensaude-Vincent's belief that objective analysis and knowledge about composition necessarily means detachment from technological uses is also questionable from historical points of view. In the second half of the eighteenth century new technological schools were founded such as the École des Ponts et Chaussées and the École Polytechnique, the mining academies and the chemical-pharmaceutical schools in France and Germany. In these new technological schools for the teaching of "useful sciences" or "applied sciences" (both are actors' terms), the teaching of analytical knowledge, mathematical and chemical, was regarded as an indispensable part of students' training. Mathematics and chemical analysis belonged to the first forms of scientific knowing and doing that were useful for technology. In the eighteenth century, knowledge about chemical composition was not only part of disinterested natural inquiry, it was also involved in the historical actors' attempts to improve certain arts and crafts such as pharmacy, dyeing and calico printing, the production of gunpowder, the making of porcelain, mining and metallurgy. Long before technological schools were established, mining assayers and assayers in the mint routinely analyzed the composition of ores and alloys. They did so no less objectively than chemists. Reliable knowledge about the composition of ores and alloys was crucial for the commercial success of mining and the money economy of a country. Therefore the eighteenth-century state authorities in Continental Europe promoted the teaching of the theory and practice of chemical analysis.<sup>22</sup>

In the eighteenth century many apothecaries and chemists objectively analyzed plants in order to acquire reliable knowledge about their composition. It was not elemental composition that stood in the foreground

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<sup>21</sup> Hacking, *Representing and Intervening*.

<sup>22</sup> Brianta, *Education and Training in the Mining Industry*.

of their analysis but rather the separation and identification of the proximate components of plants, many of which were applicable in pharmacy.<sup>23</sup> Unlike mathematical analysis, classical chemical analysis was a materially productive enterprise, and the products of chemical analysis were often transformed into useful materials. In the wake of the distinct tradition of chemical analysis that focused on proximate rather than ultimate elemental components of plants, early nineteenth-century chemists and pharmacists discovered a novel group of pure organic substances, the alkaloids. Again, their desire for objective knowledge of composition did not suppress their desire for making money. They quickly made practical use of morphine, cinchonine, caffeine and many other vegetable alkaloids they obtained in their analyses.

As is manifest in a myriad of eighteenth-century and nineteenth-century chemists' experimental reports, chemists' analyses pursued two goals: acquisition of knowledge about components as well as knowledge about the analyzed material substance itself. To the latter type of objects of study belonged not only pure chemical compounds but also mineral oil, wood, alloys, plant and animal materials, commercial dyestuffs and so on. A case in point is Michel E. Chevreul's analysis of the exotic dyestuff indigo in the early nineteenth century. Chevreul's analysis of indigo resulted in the separation of several substances that he regarded to be its proximate components.<sup>24</sup> He identified only one of these substances as the pure coloring principle (*principe colorant*), which he named *indigotine* and thus distinguished from commercial indigo. However, Chevreul, who was also director of dyeing at the *Gobelins* in Paris, did not claim that commercial indigo was no longer an appropriate object of inquiry for chemists. Far from driving a wedge between commercial materials and chemists' scientific objects, he extended his inquiries to indigo and its uses as a dyestuff. All of the components making up commercial indigo, he argued, contributed to its technical function as dyestuff. He also kept the traditional terms *matière colorante* and *extrait colorant* for denoting commercial indigo, now defined as an impure substance that was nonetheless important for chemists' practice.

Like many chemists of his time, Chevreul was a hybrid artisanal-scientific expert.<sup>25</sup> He was a savant and member of the Paris Academy of Sciences as well as a technical expert and commissioner of the French

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<sup>23</sup> Holmes, *Eighteenth-Century Chemistry*; Klein and Lefèvre, *Materials*; Tomic, *Aux origines de la chimie organique*.

<sup>24</sup> The following paragraph on Chevreul's analysis of indigo is based on Tomic, *ibid.*, 116-119.

<sup>25</sup> For his notion see Klein (eds.) *Artisanal-Scientific Experts*.

state bureaucracy. As Wolfgang Lefèvre and I have pointed out in our book, eighteenth-century and early nineteenth-century chemists did pursue philosophical and theoretical objectives, and they did study imperceptible dimensions of material substances such as affinities and composition. Yet they did not exclusively pursue these kinds of epistemic goals. In their laboratory practice chemists have been much more flexible. As the history of chemistry teaches us, they have been interested in many different dimensions of material substances, thus constituting what we have called “multidimensional objects of inquiry.”<sup>26</sup>

### **What if we Wrote the History of Chemistry from the Perspective of Chemical Engineering and Technological Chemistry?<sup>27</sup>**

In the nineteenth and twentieth centuries numerous higher technical schools were established in Europe and the US for the teaching of chemical technology and engineering. Beginning in the second half of the nineteenth century, the chemical industry also undertook efforts to establish its own research labs. Impure, mixed substances such as alloys, glass, ceramics, gunpowder, dyestuffs, woods, charcoal, mineral oil, mineral water, milk, to name only a few economically important materials, were in the foreground of chemical teaching and research in these technological institutions.

Why would we want to marginalize chemical technology and engineering in our larger picture of the history of chemistry? Why is chemistry located at modern research universities selected as the privileged point of view from which we look back at historical processes and trajectories in the history of chemistry? I have not come across good arguments for this selective focus. Chemistry never was a pure science.<sup>28</sup> It has always been an assemblage of theory and practice, science and art, pure and applied science, fundamental and applied research. Stable networks of chemical science and technology existed long before the twentieth century. Early modern chemistry was an art *and* a science, a mixed “artscience,” or, to use an analytical term, an early form of technoscience.<sup>29</sup> The sites of chemical art or practice were first mainly the

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<sup>26</sup> Klein and Lefèvre, *Materials*.

<sup>27</sup> Here I have modified Ann Johnson’s title of her excellent book review: Johnson, *What if We Wrote the History of Science from the Perspective of Applied Science?*

<sup>28</sup> Klein, *Not a Pure Science*.

<sup>29</sup> Klein, *Technoscience*.



private pharmaceutical laboratories and the metallurgical laboratories established by state authorities. In the second half of the eighteenth century chemists extended chemical practice, often with support of the state bureaucracy, to new social and technical domains such as dyeing and calico printing, the production of gunpowder, porcelain and glass. The number of specialized institutions for chemical teaching increased continually. It would be anachronistic to follow only one trajectory in the web of bifurcations and specializations of modern chemistry, namely the one ending in today's modern research universities and university teaching.

There have been additional historical types of intersections between chemical science and technology. I have already mentioned the hybrid artisanal-scientific experts who participated both in the world of artists and engineers and that of academicians. The eighteenth-century scientific academies mobilized their members in the physical and mathematical classes, among them many chemists, to evaluate proposals for innovation and to undertake technological inquiries. In the nineteenth century, many chemists teaching at universities held close personal contacts with chemical industry or they established their own chemical plants. If we paid as much attention to the concrete activities of university professors of chemistry, including their interactions with industry, as to chemical textbooks, university curricula and the disciplinary matrix of university chemistry, we should see that even university chemistry was not a pure science. Generalized statements about chemistry and its history must include chemical art and technological inquiry in the early modern period and chemical technology and engineering in the nineteenth and twentieth centuries. This implies the conclusion that modern chemistry is not merely a science of pure substances but also one of useful materials.

### **Purity in the History of Chemistry**

Any argument about purity and pure substances in the history of chemistry must take into account that the meaning of purity as well as the types of material substances involved in chemists' practices changed significantly in the history of chemistry. In order to avoid anachronistic interpretations and misunderstandings of the historical actors' concepts and practices, it is indispensable to spell out what was meant by "purity" in a distinct period and chemical culture. In the long history of chemistry, purity was an immense technical problem, but it was also a conceptual issue. I will start with a brief account of a concept of chemical purity that is strikingly different from the modern one, namely "purity" in Paracelsian

alchemy.<sup>30</sup> Apart from its historical curiosity, the case clearly demonstrates that the meaning of “purity” and “pure substance” changed in history. It further helps to illuminate historical differences in the meaning of purity that are more subtle than the difference between Paracelsian and modern chemical “purity.” A more subtle difference exists between the meaning of chemical purity in Lavoisier’s system and the modern meaning. Whereas the latter restricts chemical purity to stoichiometric compounds (apart from chemical elements); the former does not restrict it to stoichiometric compounds. I argue that Lavoisier had no modern concept of chemical purity, that is, stoichiometric purity. He rather preserved the concept of chemical purity already present in the eighteenth-century tables of chemical affinity.

### **Changing Meanings of Purity in the History of Chemistry: An Example from Paracelsian Alchemy**

The term “purity” was often used in pre-modern chemistry or alchemy. The influential seventeenth-century French alchemist and follower of Paracelsus Nicaise Le Febvre (c. 1615–1669), for example, proclaimed that “the chief ends of Chymistry,” were to “separate Purity from Impurity.”<sup>31</sup> Yet, in the context of the Paracelsian philosophy, which was widely accepted by seventeenth-century alchemists, the meaning of “purity” differed strongly from the modern chemical meaning of the term. Le Febvre’s talk about “purity” and “pure substances” must not be confused with the eighteenth-century quest for chemical analysis and the separation and identification of single kinds of chemical substances.

Referring to Paracelsus, Le Febvre proclaimed that in order to obtain a pure substance it “must be freed of that gross body wherein it is imprisoned.”<sup>32</sup> He wrote this in a chapter of his chemical treatise that is headed “Of the Pure Substances extracted out of Mixts.” The “pure substances” that Le Febvre discussed in this chapter were so-called essences, arcanas, magisteries, elixirs, tinctures and so on, all of which he regarded as “exalted” and “ennobled” by chemical art and “raised to their purity.”<sup>33</sup> He reminded his readers of Paracelsus’s argument that all of

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<sup>30</sup> There were different traditions of alchemy in the early modern period. The following account does not cover all traditions, in particular not Robert Boyle’s corpuscular approach to alchemy. It should be noted, however, that the Paracelsian alchemy was a widespread tradition in the late sixteenth and seventeenth centuries.

<sup>31</sup> Le Febvre, *A Compendious Body of Chymistry*.

<sup>32</sup> *Ibid.*, 55.

<sup>33</sup> *Ibid.*

these substances were “contained in the mystery of Nature, which he [Paracelsus] calls Purity,” and further that Paracelsus identified the body with “impurity.”

The Paracelsian concept of purity and impurity was related to distillation, and the operational distinction between the “caput mortuum” and distilled spirits. The latter were pure substances, the former impure substances. However, it would be anachronistic to restrict the Paracelsian meaning of “purity” to an operational definition. The Paracelsian concept of purity was firmly embedded in Paracelsian philosophy and the idea of an ontological hierarchy of matter, with quotidian, solid bodies at the bottom and a spiritual principle, fire or light, at the top. According to this idea, in their purest form substances were spiritualized to such degree that they acquired the nature of fire. As Le Febvre made clear, this highest stage of purity was not what chymists actually intended. For if that stage was actually achieved, experimenters were no longer able to perceive and handle a substance:<sup>34</sup>

For as Nature cannot communicate its Treasures unto us, but under the shade of Bodies, so can we do no more then to devest them by the help of Art from the grossest and most material part of that Body, to apply to our uses: for if we urge them, and spiritualize too much, so that they should flye from our sight and contact, then do they lose their bodily Idea and character, and return again to the Universal Spirit.

In Paracelsian alchemy, “purification” thus meant to free substances from corporeal qualities, to exalt and spiritualize them, and thus to bring them nearer to the nature of fire and the universal spirit.

Another curious aspect of the meaning of purity in pre-modern alchemy is its association with usefulness. Paracelsians’ claim that their art was useful, especially for medicine, was directly linked with their philosophical concept of purity. The argument was that essences, elixirs, magisteries and similar pure substances occupied a middle place in between the quotidian, impure raw substances and the pure sublunar spirits that were deprived of any corporeality. As they were freed from the rough corporeal qualities of ordinary substances they were more subtle and thus could penetrate the human body more easily. Hence they were more effective remedies than the ordinary raw materials or “simplicia” used in traditional Galenic medicine. Le Febvre claimed that:

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<sup>34</sup> Ibid., 34f.

By purity we will understand, all what in the Mixt or Compound can be found *to serve our end and purpose*; as to the contrary, *by impurity all what opposeth it self and contradicts to our intention* in the work.<sup>35</sup>

Whereas chemical purity in the modern chemical sense can be easily lumped together with objectivity and disinterestedness, this would be difficult with respect to Paracelsian alchemy. Here purity was directly and explicitly linked with pharmaceutical usefulness of the chemically prepared substance.

### Chemical Purity in the Eighteenth Century

The early eighteenth-century chemists did not explicitly reject the pre-modern Paracelsian concept of pure substances. It rather faded away along with the entire ontology and epistemology of Paracelsian alchemy. In the eighteenth century a pure chemical substance usually meant one kind of substance in distinction to an apparently homogeneous mixture of different substances. In E. F. Geoffroy's table of chemical rapports from 1718, this new meaning is clearly represented. As I have shown elsewhere in detail, the substances represented in his table were a very distinct group of kinds of substances, all of which could be individuated and identified on the basis of certain empirical regularities: they could be composed and decomposed in a distinct order that became manifest in displacement reactions, and they formed, simple binary compounds.<sup>36</sup> Furthermore, a compound that underwent reversible compositions and decompositions in a distinct order was distinguished from a mere mechanical mixture by virtue of chemical rapports or affinities between its components.

However, as Wolfgang Lefèvre and I have also argued in detail in our *Materials in Eighteenth-Century Science*, not all substances studied in eighteenth-century and early nineteenth-century chemistry displayed this type of chemical behavior. On the contrary, almost all plant and animal substances, many raw minerals, and many commercial materials that chemists studied in their laboratories behaved in different ways. Well into the nineteenth-century chemists often disagreed in their classificatory judgments. It was often difficult to decide whether samples of a plant material that were bought from different merchants and differed in smell and color, but reacted in similar ways with certain chemicals, were mere varieties of one and the same kind of plant substance or different kinds of

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<sup>35</sup> Ibid. 50; my emphasis.

<sup>36</sup> Klein, *Verbindung und Affinität*; Klein, *Material Substances*.

plant substances.<sup>37</sup> Chemists were confronted with the same type of problem as eighteenth-century botanists when they wanted to distinguish species of plants and local varieties of one and the same plant species. Similar problems existed in animal chemistry and to some extent also in the chemistry of natural minerals and mineralogy. In an essay on late eighteenth-century chemists' study of milk, Barbara Orland has provided a compelling example for this recurrent problem in animal chemistry. Chemists struggled to find an answer to the question of whether cow's, horse's, goat's and human milk were mere varieties of the same kind of chemical substance or different chemical species. As they also asked whether human milk from different individual women was the same kind of chemical substance or not, their chemical analysis of milk became directly relevant for a political discourse on wet nursing during the French Revolution.<sup>38</sup>

As a consequence of the broad range of materials studied in eighteenth-century chemistry, chemists' methods of identifying varieties and kinds of chemical substances differed greatly. Hence their concept of chemical purity (meaning one kind of a substance) referred to substances that were set apart later in the nineteenth century, namely to simple substances that were not yet decomposed, stoichiometric compounds, non-stoichiometric compounds as well as to mixtures and organic materials that merely appeared to be homogeneous based on the available analytical techniques. It was only the classes of pure chemical substances assembled in tables of chemical affinity and in the *Méthode* that were operationally defined as pure kinds of chemical substances. Based on their operational method of individuating and identifying pure chemical substances—substances that could be involved in reversible decompositions and recompositions, or analysis and re-synthesis, directed by affinities—chemists achieved agreement about the question of what were true kinds (or species) of chemical substances and what were mere varieties of one and the same chemical kind or what were mechanical mixtures. Chemical composition became the main criterion for the identification of a kind of pure chemical substance. This type of agreement did not exist in plant and animal chemistry and all other chemical domains where an operational, chemical definition of chemical purity was missing. The pure chemical substances presented in the eighteenth-century chemical tables thus constituted a stable scaffolding of chemical kinds in the midst of an ocean

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<sup>37</sup> For the latter see Klein and Lefèvre, *Materials*, 273-83.

<sup>38</sup> Orland, *Enlightened Milk. Reshaping a Bodily Substance into a Chemical Object*.

of varieties of natural and artificial substances, which often differed only in small degrees.<sup>39</sup>

To sum up, almost a century before the so-called chemical revolution, chemists began to group together, and thus to highlight, certain kinds of substances which later would be recognized as chemical elements and truly pure, namely stoichiometric, chemical compounds. In addition they also studied many other materials. This did *not* change in the so-called chemical revolution. Well into the nineteenth century, chemists even analyzed organized parts of plants and animals such as fruits, seeds, blood and nails. They also analyzed non-stoichiometric compounds and mixtures such as ceramics, alloys, milk, mineral waters, liqueurs, gunpowder, soil, ink.<sup>40</sup> In each of these cases not only knowledge about the simpler ingredients of a mixture and proximate components of an organized animal material were the goal of chemical analysis but also knowledge about the material to be analyzed.

### **Lavoisier had No Modern Concept of Chemical Kind and Purity**

In their famous *Méthode de nomenclature chimique* (1787), Lavoisier and his collaborators highlighted the same type of pure chemical substances that had already been highlighted in affinity tables. They further provided semi-quantitative information about elemental composition. An example is their distinction between *acide sulfureux* and *acide sulfurique*, which differed quantitatively in their relative proportion of oxygen. Yet in their *Méthode* Lavoisier and his group did not identify and demarcate kinds of chemical substances in a precise quantitative fashion. In their understanding information about the predominance of a distinct element, say oxygen, in two different compounds made up of the same elements (say sulfur, hydrogen and oxygen) was sufficient to clearly demarcate the two compounds from each other. It is thus not accidental that Lavoisier and his group included alloys in the table attached to their *Méthode* as well as non-stoichiometric plants substances. Furthermore it is not accidental that the Lavoisierian chemistry did not introduce chemical formulas for identifying and demarcating different kinds of chemical

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<sup>39</sup> For excellent discussion of the concept of 'pure chemical substance' involved in the eighteenth-century affinity tables see also Chalmers, *Concept of Chemical Compound*.

<sup>40</sup> All of these examples are studied in the contributions to Klein and Spary (eds.) *Materials and Expertise*.

substances consisting of the same elements.<sup>41</sup> The new Lavoisierian nomenclature neither represented exact, invariant quantitative composition nor rested on this kind of quantitative law-like knowledge.

The upshot of this is that Lavoisier had no modern concept of pure chemical substance based on stoichiometry. On the one hand, this is almost a trivial historical fact, since it is well known that “stoichiometry,” the study of quantitative laws of chemical composition, was developed after the “chemical revolution.”<sup>42</sup> The famous controversy between Proust and Berthollet about the question of whether all kinds of chemical compounds have an invariant characteristic quantitative composition took off as late as 1803. What was known long before ca. 1800 was the phenomenon of saturation. But saturation also applies to several non-stoichiometric compounds, most notably to solutions (of water, alcohol etc.) and to alloys, included in tables of affinity. On the other hand, the experts on Lavoisier have not asked the question of what the latter fact meant for Lavoisier’s concept of purity and pure chemical substance. From hindsight, and only from hindsight, the majority of the compounds included in the *Méthode* were stoichiometric compounds. However, as we have pointed out in our scrutiny of the chemical table included in the *Méthode*, it also included alloys, and in an appendix a number of mixed vegetable materials. Both alloys and several of the vegetable substances (such as tinctures) were known to vary in their quantitative composition; they were clearly non-stoichiometric compounds. Lavoisier and his collaborators thus included both non-stoichiometric and stoichiometric compounds in their table of nomenclature.

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<sup>41</sup> For a more detailed demonstration see Klein and Lefèvre, *Materials*, 247-250, 266-71.

<sup>42</sup> See Mauskopf, *Crystals and Compounds*.

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# **PRACTICAL APPROACHES**

# WHAT IS A SCIENTIFIC CONCEPT: SOME CONSIDERATIONS CONCERNING CHEMISTRY IN PRACTICAL REALIST PHILOSOPHY OF SCIENCE

REIN VIHALEMM

I wish to make three points in this paper: (1) to emphasize the relevance of chemistry to analysing science as a special kind of socio-historical practical activity; (2) to explicate the structure of a scientific concept, its meaning (sense) and reference; (3) to discuss a concrete example from chemistry—the concept of *chemical structure* in the classical chemical structure theory.

## **1. The Relevance of Chemistry to Analysing Science as a Special Kind of Socio-historical Practical Activity**

In my previous papers, I have argued that the relevance of chemistry to the philosophy of science lies not in the supposed peculiarities of chemistry **as a science** but in the fact that, within the framework of post-Kuhnian history and philosophy of science, chemistry offers certain advantages for the philosophical understanding of the nature of science.

Chemistry “as a science” should be stressed here because, as I have also argued (most recently in Vihalemm 2007, pp. 223-234), chemistry has actually a dual nature. On the one hand, it is science in the specific, narrow sense of the term, namely a physics-like science that I describe by a theoretical model called *φ-science*; it is constructive-hypothetico-deductive by its nature. The aim of *φ-science* is to examine reality from the viewpoint of laws of nature. Examining reality from such a viewpoint presupposes the construction of models as experimentally substantiated idealizations. On the other hand, chemistry is natural history, thus being a classifying-historico-descriptive discipline.

I think that the premises and limits of science, in the narrow sense of the term, were already distinctly recognized by Immanuel Kant. I mean his famous “Copernican revolution”. These Kantian ideas I would like to

interpret in my own context of practical realist philosophy of science. It is *φ-science* wherein we can suppose that objects must conform to our knowledge (in the Kantian sense), not our knowledge to objects. I reject, however, Kant's apriorism with its presupposed, fixed and immutable prior principles, and his transcendental idealism. The knowledge as well as the knower and the world that is known are all formed in practice (i.e. in human activity as a social-historical, critically purposeful-normative, constructive, material interference with nature and society producing and reproducing the human world—culture—in nature). To speak about the world outside practice means to speak about something indefinable or illusory. It is only through practice that the objective world can really exist for humans. Therefore, knowledge must be regarded as the process of understanding how the world is formed in practice, of how it becomes defined.

From the viewpoint of ordinary realism this may seem as giving up realism and the knowability of the world, as acceptance of Kant's view that the objective world, independent of the subject, remains a "thing-in-itself"; the only world accessible to knowledge is the empirical one formed by the subject in the process of cognition. But the role of practice is, in principle, different from how Kant sees it. Proceeding from practice means that it is senseless to talk of the objective world as some unknowable "thing-in-itself"; instead, we should say that the world appears as a "thing-for-us". The world-in-itself is an empty abstraction that makes the objective world indefinable since any contact with the subject is excluded.

So, there are no subjects or objects of cognition that were "ready-made" or "given" by nature itself; both subjects and objects have a historico-cultural character. Nevertheless, we can distinguish between the objects of *φ-science* and the objects of *non-φ-science* (or natural history). The former ("free falling bodies", "electric current", "light-rays", and the like) are constructed in scientific practice whereas the latter (plants, minerals, animals, and the like) are "given" to the researcher, in some way or another, by some kind of pre-scientific (or non-scientific) practices.

Alexander Bird has called pre-Kuhnian philosophy of science the "Old Rationalism"; for post-Kuhnian thinking he uses the term the "New Paradigm", to honour Kuhn's most famous notion (Bird 2000, pp. 3-7). Kuhn himself spoke of "aprioristic rationalism", meaning that it proceeds from the concept of rationality that has been borrowed from philosophy, not derived from actual science. The New Paradigm is primarily about taking seriously the actual science. It emphasises that science is not merely a logical, verbal and mathematical system; it is created by human agents, scientists, who belong to a wider specialist community and operate in a

specific system or “world” with its characteristic mental and material cultures—in a “paradigm”. So the New Paradigm basically means—as emphasised by Joseph Rouse—that science is construed as a field of practices rather than a network of statements (Rouse 1987, p. 26; 2003, p. 116).

It should be noted, however, that although it seems justified to speak about pre-Kuhnian and post-Kuhnian history and philosophy of science and to interpret Kuhn’s account of science in terms of paradigms as practice-based, this does not mean that Kuhn himself elaborated such a viewpoint and is to be clearly associated with it. One has to agree with Joseph Rouse’s claim that

Thomas Kuhn’s *The Structure of Scientific Revolutions* has also been perhaps the most misunderstood. In particular, the depth of his criticism of the representationalist epistemology has often been overlooked. Kuhn has most commonly been read by philosophers as someone who ascribes a leading role to theory in science, who emphasizes the noncumulative character of theory change, and who denies the possibility of nonneutral criteria for assessing the cognitive worth of such changes (Rouse 1987, p. 26).

And it is well known that Kuhn himself wrote in *Reflections on my Critics* that he “is tempted to posit the existence of two Thomas Kuhn. Kuhn<sub>1</sub> is the author of ... *The Structure of Scientific Revolutions* ... Kuhn<sub>2</sub> is the author of another book with the same title” (Kuhn 1970b, p. 231). Rouse says that Kuhn’s ideas should be developed “further in the direction of an account of science as practice than he himself would be happy with” (Rouse 1987, p. 27). Also, I agree with Alexander Bird in that:

in important respects Kuhn failed to break entirely with the preceding tradition. From the naturalistic perspective that has developed in “core philosophy” during the last two to three decades, which in due course spread to the philosophy of science, Kuhn’s views are shot through with commitments to the Cartesian and empiricist traditions he saw himself to be rejecting. Furthermore, I argue that it is only *partial* rejection of positivism and empiricism that explains the radical appearance of the Kuhnian viewpoint—incommensurability, the conception of progress, the rejection of the concepts of truth and verisimilitude and, arguably the world change thesis, are consequences of positivist and empiricist views that Kuhn retained (Bird 2000, p. x).

Bird thinks that Kuhn’s later philosophy developed in the wrong direction:

Kuhn ... started out with a strong naturalistic streak ... in order to build his accounts of scientific change and the nature of observation and scientific thought. But by the 1970s, Kuhn's work had taken on a much more purely philosophical, *a priori*, tone. [...] I suggest, nonetheless, that Kuhn's most valuable contribution is to be found in *The Structure of Scientific Revolutions* and not in his later work, and that the naturalistic direction of the former ... deserve[s] further study (Bird 2002, p. 443).

As said before, chemistry is an excellent example for analysing science as a special kind of socio-historical, practical activity, and for elaborating a practical realist philosophy of science. According to practical realism it does not follow from the fact that the world is accessible for science through paradigms in the Kuhnian sense, interpreted in its turn as practices developed by scientists, that we are “world makers”: these practices are the ways we are engaged with the world and allow the world to show how it can be identified in its own possible “versions”. In this context, it is worth pointing out that the development of Kuhn's views took place in close contact with chemistry and chemists. First, let us consider how he describes his shift from theoretical physics to history and philosophy of science in the *Preface* to his *The Structure of Scientific Revolutions* (Kuhn 1970b, p. xi):

It was James B. Conant, then president of Harvard University, who first introduced me to the history of science and thus initiated the transformation in my conception of the nature of scientific advance. Ever since that process began, he has been generous of his ideas, criticisms, and the time—including the time required to read and suggest important changes in the draft of my manuscript. Leonard K. Nash, with whom for five years I taught a historically oriented course that Dr. Conant had started, was an even more active collaborator during the years when my ideas first began to take shape, and he has been much missed during the later stages of their development.

Kuhn dedicated the first edition of his *The Structure of Scientific Revolutions* to James B. Conant, “who started it” (see the title page of the 1962 edition). James Conant, a chemist, who, among other things, studied the eighteenth-century chemical revolution, published a book entitled *On Understanding Science. An Historical Approach* (1947), which clearly is an important starting point for Kuhn's account of science. Leonard Nash, too, is a well-known chemist, historian of chemistry and philosopher of science, who views science as practice. In a recently published article, Jacobs (2010, p. 333) says about Nash:

As with Conant (and Kuhn) ... Nash's object ... was to describe and analyze *actual* scientific practice and knowledge, disparaging philosophers' decrees of method rules for research and their studies of the logic of 'ideal' science as futile scholasticism.

They all—Conant, Kuhn and Nash—were influenced by the thoughts of one more chemist turned non-traditional philosopher of science, Michael Polanyi. Thus it can be said that, in many ways, the New Paradigm in philosophy of science emerged on the basis of chemistry. When Roald Hoffmann asks in the title of his paper (2007, p. 321): “What might philosophy of science look like if chemists built it?”, one should better admit that, in a certain sense, chemistry *had* already greatly influenced the major change in the philosophy of science, the turn from the Old Rationalism to the Kuhnian New Paradigm. In this connection, we can see the new tendency to study science as it is actually practiced, or was practiced in history; and also, the tendency to explore the nature of sciences other than theoretical physics and to pursue other goals besides the logical reconstruction of physical theories—usually, it has been classical physics which has served as the traditional source of the philosophers' image of science. In this new situation, “philosophy of chemistry has become somewhat of a “hot” research area”, as remarked in *The Blackwell Guide to the Philosophy of Science* (Machamer and Silberstein 2002, p. 10).

In my earlier papers, I have discussed the specificity of science on the example of chemistry focusing on such general categories as *scientific theory* and *laws of nature*. In this paper I will consider the category of *scientific concept* (earlier, I have analysed the concept of concept in two papers which were published in Russian—Vihalemm 1974—and in Estonian—Vihalemm 1979). In the case of a scientific concept—which is the central element through which the scientific understanding of the world is achieved and expressed—it becomes especially clear that science should be understood as a field of practice rather than a network of statements.

I will start with a statement by the late Stephen Toulmin (1922-2009) that may sound a little surprising: “The term *concept* is one that everybody uses and nobody explains—still less defines” (Toulmin 1972, p. 8). He continues:

For many twenty-century philosophers, indeed, concepts provide their central subject matter, their very bread and butter. [...] Many of them would even describe the central task of philosophy itself as being that of conceptual analysis. Yet ... the precise meaning of terms ‘concept’ and ‘conceptual’ is rarely made explicit and frequently left quite obscure. As it

was for St. Augustine with time, so it is for them with concepts: they know perfectly well what concepts are, just so long as nobody asks them to *say* (Toulmin 1972, p. 8).

Toulmin believes that the scientific use of concepts might be compressed into the single epigram: *Every concept is an intellectual micro-institution* (Toulmin 1972, p. 166). He was actually one of the early critics of the Old Rationalism. His first book in philosophy of science was *The Philosophy of Science. An Introduction* where he emphasized the importance of paying “sufficient attention to the actual practice of scientists” (Toulmin 1967, p. 11). The first edition of this book was published in 1953, so there is good reason to include him among the founders of the New Paradigm. Toulmin stresses that rationality should not be equated with logic, and the development of science is not identical with the development of logical, verbal and mathematical systems, although such attitudes have dominated in philosophy of science:

Ever since the ancient Greeks fell in love with geometry, philosophical thought about the nature of knowledge has been dominated by models derived from mathematics and theoretical physics. [...] [I]t has tempted philosophers to concentrate questions on logical form, to the neglect of questions about rational function and intellectual adaptation. [...]

[I]n science and philosophy alike, an exclusive preoccupation with logical systematicity has been destructive of both historical understanding and rational criticism. [...] Men demonstrate their rationality, not by ordering their concepts and beliefs in tidy formal structures, but by their preparedness to respond to novel situations with open minds ... (Toulmin 1972, pp. vii-viii).

Speaking about the relationship between scientific concepts and explanation, Toulmin says that it should be understood in terms of the procedures and techniques of acting scientists:

We must ... reverse this philosophical relationship, between explanatory arguments and the activity of explaining. As we use them here, the terms ‘explain’, ‘explaining’, and ‘explanation’ will refer primarily to a range of human activities, which may or may not include the setting-out of formal, demonstrative arguments; the terms will apply only secondarily to the arguments which enter into these explanatory activities. In our primary sense, for instance, it is physicists who ‘explain’ physical phenomena, not physics. A physical law or theory can then be spoken of as ‘explaining’ phenomena only in a derivative sense, meaning that the law or theory is one which physicists successfully invoke when ‘explaining’ the phenomena in primary sense. On this interpretation, the argument itself will no longer be the ‘explanation’ of a phenomenon; at best it can ‘serve



as' an explanation when produced in the appropriate context and applied correctly (Toulmin 1972, p. 157).

## 2. The Structure of a Scientific Concept, its Meaning (Sense) and Reference

In formal logic associated with philosophy of language, the structure of a concept was analyzed by Gottlob Frege (1848-1925). It should be noted, however, that in mathematical logic one can speak about terms and predicates but not about concepts. (As an aside: there is a recent publication within the discourse of analytic philosophy entitled "The pleonasticity of talk about concepts" (Barber 1998); i.e. "concept" is here considered to be redundant.) It is interesting that Frege was criticized by Toulmin as a representative of the absolutists, an adherent of the cult of logical systematicity. Toulmin writes (1972, p. 53):

The absolutist treats the actual diversity of men's concepts and beliefs as a superficial matter, behind which the philosopher must find fixed and enduring principles of rationality, reflecting pure, idealized forms of concepts. [...]

Our representative absolutist is Gottlob Frege, whose writings did as much as anything to revive the "mathematicizing" approaches of the Platonist tradition around 1900, and did so—quite explicitly—as a means of protecting philosophy from subordination to the facts of history and psychology.

As it is well known, Frege thinks of a concept as the reference of a predicate, which is an "unsaturated", incomplete expression, in the same sense that a mathematical expression for a function is incomplete. So, we may say that, in predicate logic, a concept is expressed by a propositional function  $F(x)$  such that the outcome of substituting concrete values (objects) for  $x$  is a true proposition. Frege emphasises that "a concept [which is the reference of a predicate—*R.V.*] must ... always be distinguished from the object [which falls under the concept, or in other words, which turns the propositional function expressing this concept into a proposition with truth-value "true" —*R.V.*]" (Frege 1960, p. 44) and that "an object is something that can never be the whole reference of a predicate" (ibid., p. 48). Also, Frege distinguishes the sense (*Sinn*) of an expression from its reference (*Bedeutung*). It should be noted that Frege's *Sinn* ("sense") has also been translated as "meaning" and Frege's *Bedeutung* (whose natural English equivalent is "meaning") should then be translated as "reference". I prefer this latter terminology (i.e. "meaning")

or, synonymously, “sense” for Frege’s *Sinn*, and always “reference” for Frege’s *Bedeutung*), which seems to convey Frege’s intentions more adequately. This distinction between meaning and reference is made, because two expressions might have the same reference (both “the Evening star” and “the Morning star” denote the planet Venus), but present it in different ways, i.e. have different meaning. This distinction concerns not only proper names, or singular terms. Frege says in his “Comments on *Sinn* and *Bedeutung*” (Frege 1979, p. 118):

The same distinction can also be drawn for concept-words. Now it is easy to become unclear about this by confounding the division into concepts and objects with this distinction between sense and ... [reference], so that we run together sense and concept on the one hand and ... [reference] and object on the other. To every concept-word or proper name, there corresponds as a rule a sense and a ... [reference], as I use these words. Of course in fiction words only have a sense, but in science and wherever we are concerned about truth, we are not prepared to rest content with the sense, we also attach a ... [reference] to proper names and concept-words; and if through some oversight, say, we fail to do this, then we are making a mistake that can easily vitiate our thinking. The ... [reference] of a proper name is the object it designates or names. A concept-word ... [refers to] a concept, if the word is used as is appropriate for logic.

The sense of an expression determines, according to Frege, the thought expressed by the sentence, whereas reference determines its truth or falsity. For Frege, not only references are public and objective, but thoughts and senses as well; i.e. he adheres to a certain kind of Platonism. But Platonism, and even the Old Rationalism, are not really viable alternatives in philosophy of science any more. So, instead, let us try to develop an understanding of the structure of a scientific concept from the perspective of practical realism. Here, it seems possible to apply Frege’s semantic ideas, in a sense. We can so-to-say read them in a practical realist way, in terms of the procedures and techniques of acting scientists, as it was put by Toulmin, i.e. to bring these ideas from the Platonic heaven of pure thought and mathematically rigorous language to scientific life and practice.

To say it a bit differently, for Frege, and for logic and philosophy of language in general, concepts and objects (and actually language and logic as well) are given non-problematically, whereas for the practice-based philosophy of science the nature of scientific concepts and objects of reality, the ways how they are constructed in science, are the main topic of research. So, what is a scientific concept, and what can we say about its meaning and reference?

Earlier in this paper, I noted already that a scientific concept should not be understood merely as an element of language, a constitutive part in the structure of a proposition or a propositional attitude (in which case talk about concepts may prove to be pleonastic, as said); instead, it should be seen as the central element through which the scientific understanding of the world is achieved and expressed—"an intellectual micro-institution", to recall Toulmin's epigram. Let us, however, limit our analysis here and focus mainly on the structure of a scientific concept in the linguistic sense—on its meaning and reference. In philosophy of chemistry and in general philosophy of science, there has been much discussion of this issue, especially in terms of the "problem of natural kinds". I think that a great part of the confusion concerning natural kinds in philosophy of science is related with this inadequate context: the problem of natural kinds should not be seen, in the context of science, as the problem of the reference and meaning of corresponding **terms**, but as the problem of the reference and meaning of corresponding **scientific concepts** (see also: Vihalemm 2003b). Rom Harré puts this point very well in his book *Varieties of Realism*: "'Terms denote; people refer.'" I owe this crisp formulation ... to Mary Tiles. Referring is a human activity and reference is an achievement" (Harré 1986, p. 124).

In my view, the reference of a scientific concept should be seen in the following way. It is a certain abstract object, an idealized construction that is a model of a certain actual system given through practice. The meaning (sense) of the concept lies in the referring activity, in the procedures by which the reference is found and the relevant abstract object constructed. It involves the understanding of the role of certain real objects and phenomena, their relations, functions, characteristics, the ways they are handled in a certain system of human activity, i.e., in scientific practice. The concept is like a scheme for constructing, creating or recreating something.

This can be illustrated with an example from Spinoza: what is a circle? Instead of defining it formally "as a figure, such that all straight lines drawn from the center to the circumference are equal", we should, according to Spinoza, "explain the essence of a circle", that is, we should explain how to construct it—as "the figure described by any line whereof one end is fixed and the other free" (Spinoza 1677).

Or let us take another example from everyday life—the concept "house". What provides the basis for this concept? Why is it so that, after having acquired the concept of a house, we are able to recognize a house in very different entities (a farm house, a skyscraper, a mud hut, and even the photos, drawings and paintings of these)? We never see a house *as*

*such*. The reference of this concept is not a real house (which is always concrete), but a certain abstract object, scheme, construction, model, that is identified proceeding from the meaning of the concept. The meaning of the concept “house” involves such things as the purpose for which the house is built, the way how it is constructed etc. For example, since a house is built in order to protect people from unfavourable weather conditions, it has to be constructed so that it has a roof and walls, or the roof has to be built in such a way that it would also substitute for the walls so that people could live under it.

Here, a question may arise. What about the objects that are not built by man, but are so-to-say built by the nature itself—for example, a dog? The same principles seem to apply in this case as well since we see nature also through the prism of socio-historical activity. In that sense—and to such degree as we understand it on the conceptual level—a dog, too, is “constructed” by us, and according to the same principles as a house. The difference lies only in the fact that we do really build houses, but we do not really build dogs (at least for now!), we construct them only in our thought and imagination, which is why it remains largely, to use Kant's terminology, a “thing-in-itself” and becomes (if it becomes) a true thing for us only when we can recreate it with all its dog-like qualities (cf: Boroday 1966, pp. 92-107).

Every non-created thing is reproduced in a concept as a thing created. In a concept, we reproduce our human, practical, sensuous-objective activity in the form of objects of reality. And *vice versa*—objects of reality are reproduced in a concept in the form of human, practical, sensuous-objective activity (cf: Arsenyev, Bibler, Kedrov 1967, p. 67). It is a fundamental mistake to search for an objective world “in itself”, i.e. to consider reality outside human activity, to look for an object which would directly “correspond” to the concept. There is no such real object; there is only the acquired (or constructed) abstract object, the model of the “real object”. Every object, every fragment of objective reality is—strictly speaking—inexhaustible, having innumerable aspects and connections with the rest of the world. However, in a certain system of human (cognitive) activity only certain aspects of this real object are isolated that are especially important from the viewpoint of this particular activity.

In science, the main form of practice is scientific experiment. We can distinguish between empirical and theoretical concepts and objects. Empirical concepts, and the corresponding objects, are created by schemes of real experiments. Empirical objects, too, are abstract in the sense that they, although put into correspondence with real objects in experiments, cannot be identified with those objects (as said, they are inexhaustible) and

are defined only via characteristics that are important in the particular experiments. As for theoretical objects, they are constructed through the process of idealization and are even less directly identifiable with real objects because they may have characteristics that the real objects entirely lack. For example, *point masses* are zero-dimensional objects having only one characteristic (mass), though this does not render them altogether unreal or fictitious. A point mass does really exist in the sense that in certain conditions, from the viewpoint of certain connections and relations (which are established by classical mechanics), real objects (and not certain specific things that are called “point masses”) do indeed behave as point masses—their dimensions prove to be irrelevant.

A scientific concept reflects in its abstract object the characteristics of a certain object or aggregation of objects of some real system. These characteristics enable it to serve as a model of some real system in a certain scientific paradigm without contradicting the facts. So, for example, such theoretical concepts as “phlogiston”, “aether”, and “caloric” were in accordance with facts available to the science of the time. Nowadays, these concepts are no longer accepted, but not because there are no facts to prove their existence—these were lacking earlier, too!—, but because nowadays these concepts contradict the facts that were not available to the earlier scientific paradigms. The concept of phlogiston is quite interesting from the viewpoint of practical realism. I have discussed it from a somewhat different perspective in an earlier paper (Vihalemm 2004, pp. 46-54).

A few things should be said on the issue of the definition of concepts. It goes without saying that, from the viewpoint of a practice-based account of concepts, verbal definitions of concepts usually do not matter much, not to speak about concepts being created by definitions—a view occasionally defended by some. (In axiomatic formalized systems, concepts have to be treated somewhat differently because in such systems formal, precise definitions of concepts are indeed necessary.) The concepts of natural sciences obtain their definitions through a system of knowledge which emerges in practical activities characteristic to the science involved—those systems of activities having been described by Kuhn as “paradigms”. Concepts emerge together with the corresponding theory. We have seen that the reference of a scientific concept is a certain abstract object as a model. There is good reason to think of scientific theories as based on models as well (Giere 1988; 2000).

On the one hand, a concept turns out to be a concentrate of a theory, so-to-say; in order to “define” it adequately, one has to construct and present a theory of the phenomena involved. On the other hand, it is

merely an element in a theory—the latter being a whole sophisticated system of concepts (and of the corresponding models). The most basic and elementary system of concepts is a pair of concepts. In this sense, the most basic conceivable theory is a principle or a law; this principle or law then expresses the relationship between the two concepts (and the corresponding models). Consequently, the simplest way for defining a concept through a theory is defining it via a principle or a law. For example, the concept of a *chemical element* gets its definition through the periodic law of elements as a definite *position* in the periodical system based on that law (Arseniyev, Bibler, Kedrov 1967, pp. 340-435; Vihalemm 2003a, pp. 12-20).

Next, to illustrate this general account I shall consider a particular example of a chemical concept—the concept of *chemical structure*, within the context of the corresponding theory (the classical theory of chemical structure).

### 3. The Concept of *Chemical Structure* and the Classical Theory of Chemical Structure

In the following, I will rely on Ronald Giere's constructive-realist, model-based conception of scientific theory (Giere 1988; 2000).

In developing his theory, Giere has explicitly referred to Thomas Kuhn (1970a), whose paradigms, in the narrow sense of the term, as shared examples, are also non-linguistic entities: it is exactly these entities that play a central role in understanding the functioning of both scientific theory and science in general. The main emphasis is on analyzing the scientist's activities, the practices specific to science. Among other things, this means that it has become rather difficult, in philosophy of science, to stick to the comfortable distinction between the “context of justification” and “the context of discovery”, and let philosophy of science deal with the first of these only.

When speaking of a scientific theory in general, one should surely be aware that the scope of philosophy of science has widened remarkably in recent times. As said already, it has drawn closer to the actual practice of science, to the science “in the wild”. Social, historical and anthropological aspects have all gained importance and there is interest in nearly everything that is done under the name of science, or that has been done under this name earlier in history; e.g., philosophers now take more of an interest in those disciplines where mathematics is not applied and where no formal theories are constructed (or, at least, such theories have not been of central significance). Nevertheless, I think that this is not an obstacle to developing

a concept of a certain narrower, physics-like science, and to working out a more general theoretical model for understanding science.

In my opinion, Giere's model-based conception is essential for understanding scientific theory as a general category of philosophy of science (Vihalemm 2009). According to Giere (1988, p. 82):

There is ... no direct relationship between sets of statements and the real world. The relationship is indirect through the intermediary of a theoretical model...

Of course, assertions about the existence of similarity relationships between models and real systems do require theoretical hypotheses, which are indeed linguistic entities. But for these a 'redundancy theory' of truth is all that is required ... And there is a truth relationship of the correspondent type between the statements characterizing an abstract model and the model itself. But this correspondence, which reduces to definition, is not a problem. The relationship that does the heavy representational work is not one of truth between linguistic entity and a real object, but of similarity between two objects, one abstract and one real. From this point of view the difficulties with the standard view arise because it tries to forge a direct semantic link between the statements characterizing the model and the world—thus eliminating the role of models altogether.

In the context of the current paper, I would like to draw attention to the fact that according to Giere, a scientific theory is not a well-defined entity. For instance, classical mechanics is not, nor has ever been, in actual scientific practice, merely an axiomatic system, a collection of propositions whose core is given by Newton's three laws and the law of gravity. This, however, has been the general and also philosophical understanding. According to this understanding, Newton's theory with its central laws has been understood as directly applicable to the world, and the central emphasis was placed on finding out whether this theory and its universal laws are true, either from the viewpoint of realism or empiricism (realism has mostly been empiricist). According to Giere, the central role in scientific theory belongs to models, idealizations, and it is precisely to these that the theoretical concepts and laws directly apply.

Here, I would like to emphasize that the introduction or creation of such theoretical models as idealized constructions should be experimentally substantiated. When we talk about how a theory works, or rather—how one works with a theory—, it is the handling of these models which is important; and it is not only interpreting theoretical terms on these models, or the so-to-say defining of these models which is important, but also showing from which aspects and to what extent the real systems can be identified with these models (this usually requires

sophisticated instruments and equipment). This means raising and testing of theoretical hypotheses. Only in this respect and in this phase the issue of truth comes into play.

Differently from the classical conception, this work on the models (neither the defining of models nor the identifying of the models with real systems) is not an activity which takes place within the theory itself as part of the development of the system of statements; rather, it is an activity which is practical, objective, experimental and also social. To recall Kuhn once more, there is a *paradigm*—associated with *tacit knowledge*—which is important. According to Giere, scientific theory is: “(1) a population of models, and (2) various hypotheses linking those models with systems in the real world” (Giere 1988, p. 85); “... no necessary and sufficient conditions determine which models or which hypotheses are parts of the theory” (*ibid.*, p. 86). These issues are settled by the decisions of a scientific community. Scientific laws are not statements making direct claims about the world; rather, they provide definitions of various theoretical models, or idealized systems. In classical mechanics, the latter include such constructions as the simple harmonic oscillator, the simple pendulum, the damped linear oscillator etc.

Let us now turn to chemistry and consider a typical example of chemical theory—the classical chemical structure theory. Both in classical and modern chemistry, the concept of chemical structure forms undoubtedly the core of chemical science. To cite the Nobel Prize laureate Roald Hoffmann: “Chemical structures are among the trademarks of our profession, as surely chemical as flasks, beakers, and distillation columns. When someone sees one of us busily scribbling formulas or structures, he has no trouble identifying a chemist” (Hoffmann and Laszlo 1977, p. 1).

So, one might say that chemistry can be identified through chemical structures. But the question is: why and how do these chemical structures make up the core of chemistry? When we compare the classical chemical structure theory that originates from the second half of the 19th century, from the 1860s, for instance, to classical mechanics, should we say that, in the philosophical sense, these two are equally scientific—or should we instead say that, in chemistry, the conception of scientific theory is somewhat peculiar, so that it is not, or even should not be, the same as the conception of scientific theory in physics? Such ideas have been put forward quite often. Sometimes, the chemical structure theory, and not only its classical form but also the newest versions, have been seen as insufficiently developed theories that someday might become decent scientific theories, provided they can be substantiated by the theories of



physics—nowadays deduced from quantum physics. True, this programme of reducing chemistry to physics is not popular anymore; instead, the philosophy of chemistry rather tries to emphasise and explain the peculiarity of chemistry.

Of course, it is impossible to go deeper into these problematic issues here. In the present paper, I will not consider the issue of the peculiarity of chemistry in general, but limit myself to a more specific question whether there is any reason to view scientific theory in chemistry as essentially different from a typical theory in physics. I hold that “scientific theory” as a general category in philosophy of science should be considered, in the sense of its philosophical content, an invariant notion applicable to any science (provided we are indeed dealing with a science). I cannot discuss my own concept of science here (as said, I call the theoretical model of science, which I have proposed,  *$\varphi$ -science*) but suffice it to say that, in my opinion, one surely needs some kind of a theoretical model of science in order to define a research area as science.

Seeing the classical chemical structure theory as a “normal” scientific theory is made more difficult by the fact that it is not a mathematically formulated theory, in the sense that it does not rely on any mathematical disciplines or use the language of mathematics. Of course, it has to do with mathematics in the very general philosophical sense of τα μαθηματα, as Heidegger (1977, p. 118), for instance, has pointed out, namely—a certain kind of *a priori* knowledge: “*Ta mathemata* means for the Greeks that which man knows in advance in his observation of whatever is and his dealings with things.” Also, mathematics is involved here in another sense: from the viewpoint of philosophy of science, we can say that the procedure of idealization has been applied; through human activity, practice, first of all through experiments, the relations have been abstracted from objects that are being worked with; this system of relations into which these objects enter has become the ground for their description; i.e. we do not consider real objects any more, in their real relations, but this system of relations itself as an idealized object (Gryaznov 1982, p. 64). Through this idealized object—the system of relations—the objects themselves (as explored in this system) get defined (cf. also Cassirer 1953, pp. 39, 94, 110).

The central notion of chemistry, a *pure substance*, is a typical idealization. When speaking about mathematics as the language of science, in chemistry this function is fulfilled by the language of chemical formulas (i.e. the language of structural formulas in the chemical structure theory). This chemical language is a rather strict

system, and an efficient tool for experimental activity; it is a semiotic structure that

represents substances in certain relations with each other, i.e. substances within the chemical network. [...]

... every structural formula unambiguously corresponds to certain pure substance and *vice versa*; and every modification of a structural formula corresponds to a certain chemical change of a substance, and *vice versa*. Given both a set of structural formulas and a set of rules for allowed structural modification, we are able to generate new structural formulas by applying the rules to the former ones. The outcome of such a structural modification is, per definition, a representation of a possible substance and as such subject to further structural modification according to the rules. If we translate that into the language of substances and chemical properties, it comes out that we have *predicted new substances, including its chemical properties and the chemical way to produce them*. That is exactly, how millions of new substances have been predicted and produced during the last hundred years ..., providing that the *chemical sign language is actually one of the most predictive theories of science at all!* (Schummer 1998, pp. 152, 153)

In addition to the fact that, in the process of formulating the chemical structure theory, no mathematics was applied in the usual sense, there was even no system of well-defined statements. This is, by the way, one reason why the question still remains open of who should be seen as the author of this theory (see, e. g., Rocke 1981). Mainly, but also solely according to the research by Soviet historians of chemistry, more specifically Georgiy Bykov, the sole author is Alexandr Butlerov. Butlerov was the first to briefly formulate the main principles of the theory, in his presentation to the 36<sup>th</sup> congress of German naturalists and physicians in Speyer, in 1861 (Butlerov 1861):

To be sure, we do not know what connexion exists between the relative chemical effect of the atoms inside a compound molecule and their relative mechanical positions; we do not even know whether, in such a molecule, two atoms which directly affect each other chemically are in fact situated next to one another, but we cannot deny, putting the concept of *physical atoms* entirely to the side, that the chemical properties of a body are determined in particular by the chemical bonding of the elements which form it. Proceeding from the assumption that there inheres in each *chemical* atom only a specific limited quantity of chemical force (affinity), with which it participates in the formation of bodies, I would designate this chemical cohesion, or the manner of mutual bonding of the atoms in a compound body, by the name *chemical structure*.

This familiar rule which says that the nature of a molecule is determined by the nature, quantity, and *arrangement* of its elementary components could thus *temporarily* be altered in the following way: *the chemical nature of a molecule is determined by the nature and quantity of its elementary components and by its chemical structure* (cit. from Rocke 1981, p. 35).

A justified question arises: why is Butlerov not seen by chemists or historians of science as the undisputed author of the central classical theory of chemistry? There is no reason to suggest malicious hushing-up or the like. Neither is there any serious reason to consider Bykov simply an eager Soviet patriot, boosting Butlerov, as it was regrettably done quite often those days. Bykov definitely was a serious researcher of the history of chemistry.

The question is a rather difficult one and cannot be analysed here. Among other things, it nicely illustrates the idea mentioned before—that our understanding of scientific theory proves insufficient if we regard it only, or chiefly, as a system of mathematically formulated statements, or merely as a system of statements (that is, if we hold on to the “statement view”). If we see theories as populations of models, things become much clearer. In this particular case, the chemical structures of compounds themselves are the models that Giere speaks about and which (as stressed by him) can be neither defined nor identified with real substances through purely theoretical activities such as formulating a system of statements, but are instead created through the practical, experimental and social activities of scientists. It is quite likely that, in Butlerov’s case also, Butlerov may have given a compact formulation of the principles of the chemical structure that had emerged to his time, but the Speyer presentation cannot be viewed as the birthday of a genuinely new theory of chemistry. The theory as formulated by Butlerov did nothing to improve the ways and procedures for identifying or synthesizing new compounds with particular structures: at the time of the Speyer congress, the principles of the chemical structure of substances, which had emerged in the actual practice of chemical research, had been in use for some time already. For a synthesis (or identification), a concrete method, an actual successful synthesis and experimental research into the properties of the new compound were necessary anyway. A verbal formulation has real content in chemistry only if it has a clearly delineated counterpart in experiment. This is revealed more clearly in chemistry than, e.g., in modern theoretical physics where mathematics often tends to be so autonomous that the borderline between physics and mathematics becomes hazy. In my view, the idea that “theory is considered a tool for chemical

experiments, and not the other way round” (Schummer 2004, p. 406) applies not only to chemistry, but to the relationship between theory and experiment in science generally. A scientific theory acquires the quality of being *scientific* and is anything worth at all only if it is experimentally substantiated, and if, on the basis of the theory, phenomena in the actual world can be predicted, produced and controlled.

In the organic chemistry of the 19th century, the development of concrete methods of chemical synthesis for a broad and important class of compounds received far more attention than Butlerov’s rather general theoretical formulation, which failed to offer any novel or useful information for creating particular compounds. Therefore, it is not surprising that Butlerov became world-famous not so much for his formulation of the principles of some new theory, but for the discovery of several methods of chemical synthesis and for research into the corresponding class of compounds. The principles of chemical structure emerged from the chemists’ actual experimental practice as if by themselves, without being founded on any general theoretical formulations by Butlerov or anyone else.

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# FROM CHEMICAL PRACTICES TO A RELATIONAL PHILOSOPHY OF CHEMISTRY

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## Introduction

Our enquiry deals with ways of *doing* chemistry with the view to scrutinizing patterns of “ongoing engagement” with the world, to use Rouse’s turn of phrase (Rouse, 1996). In line with Denis Diderot (1754) and the later Wittgenstein, we agree that a careful study of what people actually do within the ‘terrain’ of their activities is of importance and should be addressed by considering their specific sites and goals. In this respect, we will first query earlier and current chemical works in order to point out what is at stake when chemists synthesize, purify, and analyse a molecule or a material. In doing so, we will draw our attention to: (1) the alchemists’ transmutation, (2) the displacements of middle salt and their role during the eighteenth century, (3) the role of Mendeleev’s elements, and to (4) current chemical devices used in nanochemistry, materials science, and combinatory chemistry. We will thus consider: (1) chemical theories and representations, (2) laboratory operations, and (3) apparatus and instruments. This first part will highlight that chemists incorporate the objects that they enact by tailoring *networks of interdependencies*. Chemical bodies are *co-defined* by means of operations and chemical reactions. Analogy allows chemists to propose taxonomies that are context-sensitive and dependent on relations.

We will then return to a laboratory of research in order to study how quantum chemists achieve their calculations as regards chemical reactivity. We will emphasize that this theoretical work is utterly relational in so far as quantum chemists intertwine different models, empirical data from various instruments, chemical knowledge and know-how, and theoretical estimates in order to determine a molecular geometry or energy barrier heights. We will thus assert that both chemical bodies and chemical practices can be investigated from a relational point of view. Our approach is not to apply a relational approach developed within another area of



human thought—physics, philosophy, logic, and biology—to chemistry, but to identify the requisite contents that such a relational approach must display in order to fit chemical practices. We will then confront those requirements with the different relational forms of philosophy available—Harré and Bensaude-Vincent—in order to draw some conclusions and to develop our own perspective.

## **Chemical Practices and Relational Strategies: Historical Insights**

### **Alchemical Transmutation**

A metal was considered to be a ‘mixture’ from which alchemists could separate different basic ‘principles’ thanks to calcinations, distillations, and dissolutions. They could then recombine those principles in order to synthesize a novel substance. A wide range of competing theories of matter were at stake depending on: (1) the number of basic principles—from three to five, (2) the relative primacy of Salt, Sulfur, or Mercury, (3) the importance of theory of the ‘seeds’, and (4) on the belief in a universal ‘Spirit’ of the world (Joly, 2007). Whatever their divergences may be, those theories defined chemical bodies by means of operations. Moreover, they considered those bodies to be ‘tools’ for acting upon the world. Qualities—hot, cold, wet, and dry—were not merely opposed as it was previously the case within Aristotle’s philosophy but, on the contrary, displayed gradual and quantitative differences. Alchemists skillfully contrived new apparatus in order to synthesize new ‘mixtures’. In doing so, they made their basic principles co-exist inside a particular substance. In short, they developed relational strategies to transfer principles from one body into another. All those theories were themselves utterly relational in so far as they entangled various assumptions, representations, know-how, and goals—from medicine to metallurgy, to quote but a few domains. All those approaches cannot be encompassed within a linear and unique tradition (Principe & Newman, 2001) but should be re-evaluated as being many examples of a system of defense against the mainstream tradition originated from Aristotle and Galen (Joly, 2010). To conclude, alchemists’ transmutation can be described as a relational process based on the circulation of basic principles and embedded in networks of cultural backgrounds. Let us point out how a new framework of relations between chemical bodies emerged during the eighteenth century.

### Table “Des Rappports”: Experiments and Affinities

The new rules of the French Royal Academy of sciences (1699), Wilhelm Homberg’s work on the interchangeability of middle salts—our current neutral salts, the Newtonian philosophy influences at the end of the seventeenth century, Paracelsus and the alchemists’ traditions, paved the way for the empirical setting of affinity tables during the eighteenth century (Stengers, 1991; Bensaude-Vincent & Stengers, 1996). From Etienne-François Geoffroy (1718) to Torbern Bergman (1775), these tables were incessantly multiplied and improved. Some chemists, such as Louis-Bernard Guyton de Morveau (1773), developed the first experimental devices to quantify these affinities (Daumas, 1946; Roberts, 1991). Geoffroy began his memoir entitled ‘Table des rappports’ at the French Académie des Sciences by the following words:

One observes in chemistry certain rappports between different bodies which allow them to unite easily with one another. These rappports have their degrees and their laws. One observes their different degrees in that among several confounded matters with some disposition to unite together, one unites constantly with a certain other in preference to all others (Cited by Mi Gyung, 2003, p. 134).

Let us recall how Gabriel François Venel described the third column step by step during the 18<sup>th</sup> century:

One applies mercury to a silver dissolution in nitrous acid; this substance having more relation with this acid, than this acid has with silver, it unites to it and precipitates silver. If one decants the liquor one will have separated silver, and on the other side mercury dissolution in nitrous acid, if one adds a lead blade to this mercury dissolution, lead has more relation with nitrous acid than mercury, it unites it and precipitates mercury. If one decants it the precipitated mercury remains on one side and on the other side a lead dissolution in nitrous acid; if one adds a copper blade to this dissolution, copper has more relation with nitrous acid and unites to it, lead will be precipitated too and there remains a copper dissolution in nitrous acid; if one adds iron copper is precipitated, if one separates as must always be done, one will have the iron dissolution [...]. (Cited by Lehman, 2010, p. 21).

The word ‘relation’ immediately comes to the fore. Let us summarize the former successive chemical reactions as follows—we do not use the alchemical symbols in order to simplify our presentation:

Chemical bodies	Our symbols	Chemical reaction
Nitrous acid	A	No reaction
Iron	a	$Ab + a \rightarrow Aa + b$
Copper	b	$Ac + b \rightarrow Ab + c$
Lead	c	$Ad + c \rightarrow Ac + d$
Mercury	d	$Ae + d \rightarrow Ad + e$
Silver	e	$A + e \rightarrow Ae$

This table was consulted to validate the process for preparing a substance or for purifying a metal. Chemists compared the strength of the links between chemical bodies and used them in order to predict chemical transformations and selective displacements of metals. The explanatory function of the alchemical principles was gradually replaced by the concept of union and disunion between chemical bodies. Chemists carefully performed chemical reactions by using those tables as guides for action. One should remind that, at this period, the current word chemical ‘operation’ was used to mean what we currently call a chemical ‘reaction’ (Holmes, 1996). Moreover, a ‘chemical property’ referred to observable phenomena that occurred when a substance was heated or mixed with a reagent (Klein & Lefèvre, 2007). Chemists took into account a large variety of details including: (1) the reactant proportions, (2) the duration and the strength of heat, (3) physical properties—such as the volatility of resulting products, (4) the speed of reaction, and (5) the glassware, vessels, and furnace to be used in order to achieve a particular goal. Those tables allowed chemists to predict, to design, and to justify their experiments. They also enabled them: (1) to contrive new criteria to identify compounds operationally by using extraction, synthesis, and analysis within laboratories, and (2) to teach chemistry. According to Holmes:

Homberg’s classification of middle salts and Geoffroy’s table provided conceptual frameworks to organize and clarify knowledge of chemical substances and operations that had been accumulated over the preceding centuries (Holmes, 1989, pp. 39-41).

The tables of “rapports” thus fused a large amount of experiments into a relational scheme. Ursula Klein proposes to reinterpret the table in a consistent way by considering that the right half of the table deals with the actions of metals in the ‘solution’ of fire whereas the left half is concerned with actions in aqueous solutions. According to her, this unifying power of the table gradually entailed a new conceptualization of fire as a solvent or as an instrument rather than as an elementary ‘principle’ as it was formerly the case (Klein, 1995). In this respect, the relational scheme could be

extended from aqueous solution to gas-phase combustion. Let us draw a parallel with the 18<sup>th</sup> definition of ‘*menstrua*’—the solvents in a liquid-phase in our current terminology. In the Diderot’s *Encyclopédie*, Venel defined water as a ‘*menstruum*’ or a solvent in order to achieve dissolution that is considered to be a real blending. In this respect, Venel defined water as an exemplary solvent instantiating the general phenomenon of dissolution rather than as an individual entity considered in isolation (Lehman, 2009). The *Encyclopédie* is explicit regarding the relational definition of ‘*menstrua*’, solubility, miscibility, or fluidity, to quote but a few concepts defined operationally. They are context-relative and not intrinsic. The article entitled ‘miscibility or solubility’ clearly stated that this property is always relative in that miscibility is not embedded in any chemical bodies taken in isolation but only displayed in the presence of other ‘substances’. According to Venel, the action of the solvent upon a sample should be understood as an interaction. In this respect, one should say that water dissolves sugar as well as sugar dissolves water in so far as they are co-defined within an ordered process of combination, precipitation, or extraction. A lot of chemists during the 18<sup>th</sup> century—but not all if one remembers, for instance, Georg Ernst Stahl’s belief in intrinsic chemical powers—put the elementary principles into question. They gradually proposed an alternative relational scheme focused on the ‘*rappports*’ between bodies. In doing so, they investigated what was persisting within a chemical transformation and what was changing. Let us now explore another epistemological shift related to the notion of chemical element. This shift occurred during the nineteenth century and implied the emergence of new relational classifications.

### **Mendeleev’s Element as a Unifying Relational Unit**

William Prout’s assumption of the derivability of all the elements from hydrogen entailed the primacy of the atomic weight system as the criterion for classifying chemical elements. Following Prout’s line, researchers such as Johann Döbereiner pointed out accurate and astonishing correlations between arithmetical relations and chemical analogies within sets of three chemical elements called ‘triads’. He carried out his calculations in 1829 by using Berzelius’s values of atomic weights. Leopold Gmelin then widened the correlations from triads to larger ‘family’ of elements. The proliferation of correlations and classifications occurred after 1850 when researchers started to discover new elements and to integrate the new concept of ‘organic radicals’ into mineral chemistry. Those strategies focused their interest on local arithmetic correlations to the detriment of

global analogies between chemical properties and thus failed in classifying elements into a coherent scheme while up-to-date spectroscopic methods provided scientists with new accurate correlations (Bensaude-Vincent, 1986, 1989).

In 1860, the Congress of Karlsruhe aimed at clarifying and framing: (1) basic concepts such as molecule, atom, and element, (2) atomic weight systems, (3) nomenclature, and (4) notations. For the first time, chemists from all over the world met together in order to choose and to define common methodologies and definitions. The Gerhardt-Cannizzaro's system of atomic weight thus became the official framework despite deep divisions between atomists and equivalentists. In line with this new standard, John Alexander Newlands proposed a law of octaves (1865) while William Olding set up a whole periodic system (1865). Those classifications neither allowed them to predict new elements nor did they pave the way for accurate correlations of atomic weights (Bensaude-Vincent, 1986, 1989). Mendeleev acknowledged that this congress suggested him the idea of an overall periodicity of the elements depending on the increasing numerical value of their atomic weight. He believed in 'the peculiar individualities' of the elements and in 'the infinite diversity of the elemental individualities' (Mendeleev, 1889). He was not running after a *proto hyle* to think about the unity of the universe, but after a unique periodic law connecting the 'multifarious relations<sup>1</sup> of matter' (Mendeleev, 1889, p. 644-645). According to Mendeleev, a crucial distinction must be done between an observable *simple body* that displays chemical and physical properties and a *chemical element*, which causes those properties. This basic element possesses at least one attribute, namely, the atomic weight which served to distinguish it from the other elements and which was used to order the elements in a unique and coherent sequence (Scerri, 2005). Mendeleev stated:

It is useful in this sense to make a clear distinction between the conception of an element as a separate homogeneous substance, and as a material but invisible part of compound. Mercury oxide does not contain two simple bodies, a gas and a metal, but two elements, mercury and oxygen, which, when free, are a gas and a metal. Neither mercury as a metal nor oxygen as a gas is contained in mercury oxide; it only contains the substance of the elements, just as steam only contains the substance of ice, but not ice itself, or as corn contains the substance of the seed but not the seed itself (Mendeleev quoted by Scerri, 2005, p. 129).

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<sup>1</sup> Our emphasis.

This rupture from Lavoisier's standpoint allows him to predict some properties and the existence of other elements such as the *eka*-iodine. Mendeleev brought chemical similarities and *contrasts* to the fore and paid attention to differences between elements. He gradually construed a network of relations thanks to approximations and a careful study of available elements by means of trial and errors. He defined an element from within its *relations* with other elements. For example, the *reactions* between alkali metals and halogens allowed him to infer that they shared the same valency even if they displayed different combinations with other elements. This contrast helped Mendeleev identifying an interesting *regularity* as regards the differences of their atomic weights.

Mendeleev stated that his method consists of simultaneous interpolation within groups or columns as well as within periods or rows of the periodic table. He carried out his procedure by taking the average of the sum of the values of the four elements flanking the element in question. In doing so, he accurately calculated the atomic weight of the element selenium (Scerri, 2001, 2007). He thus gradually co-defined elements by means of their relations with other elements. Bensaude-Vincent and Simon claim that:

By assigning a place to each element, the periodic system anchors the unit-element in a whole network of material, chemical relationships (Bensaude-Vincent & Simons, 2008, p. 160).

Some groups of elements share similarities and it is always possible for a chemist to foresee a kind of reaction between elements belonging to two different columns. Element is thus a 'metaphysical notion'—an 'unobservable substance'—(Scerri, 2005) that is to say an abstract entity which secured the conservation of material individualities through chemical transformations. The element became a 'mere node' interlinked with other elements within a network of material transformations. The concept of element thus gained a strong explanatory and heuristic power. Elements can circulate, be exchanged while respecting the 'Conservation Law' (Bensaude-Vincent & Simons, 2008). Before concluding this first part, let us envisage examples as regards current chemists' works.

### **Nanochemistry and Materials Science: Function, Relation, and Interfaces**

Nanochemists and materials chemists design new molecules in order to make them play a specific and local role—a rotary movement for the molecule rotaxane, a local gradient of property for liquid crystals, and so

on. In this respect, a molecule is a piece of matter that has a *function* to play within a chemical process. Chemists functionalized a specific molecular target or a material surface to achieve a specific goal such as trapping pollutants having a definite shape or volume. In this respect, a molecule is regarded as a ‘machine’, which performs a localized action. Nanochemistry uses self-assembly synthetic methods to organize inorganic, organic, and polymeric building-units into materials with novel chemical and physical properties and unprecedented structural features that span angstrom to millimeter length scales. Materials can be synthesized by molecular and supramolecular design, self-assembly and self-organization, and crystal engineering. In a nutshell, chemists use high-selective and relational strategies to design a molecule step by step. They can follow the whole process by means of new instruments and techniques such as the two-dimensional NMR or the atomic-force microscopy. The work-scale, the apparatus, the bottom-up devices, and the energies involved are different in order to provide new specific molecular reactivity. Researchers use some instruments and the surroundings of their molecular target in order to make it play the required function. The surroundings are the medium by which chemists intervene on a molecular target. The macroscopic properties of those composite materials depend on the control of the interfacial properties at the molecular or at the nano scales. Controlling the chemistry or the physico-chemistry of those interfaces is of primary importance. As a matter of fact, this control allows chemists to modulate and to optimize the properties displayed at the macroscopic level. Temperature, time, and feeds/stoichiometry are crucial parameters to synthesize a molecule or a material. Let us just take an example extracted from the paper about interfaces proposed in the first part of the present book (Llored *et al.*, 2013).

Precipitation is a very interesting synthesis method, because of its versatility. The different steps of the process can easily be modified by the chemist, by simply changing the operating conditions. The most common are solvent evaporation, or chemical reactions that produce insoluble species. Starting from a different number of nuclei, particles will grow to attain different final sizes and morphologies; thus by adding a reactive chemical at once or in a continuous way, the final materials may appear completely different. By adding a small amount of fine material to be precipitated-seeds, the apparently chaotic nucleation step can be better controlled. For example, adding calcite seeds allows the precipitation of pure calcite, whereas a mixture of calcite and vaterite with a larger particle size distribution and various morphologies are obtained without seeds (Figure 1).

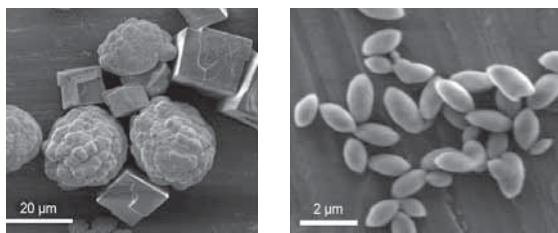


Figure 1: (Left)  $\text{CaCO}_3$ : mixture of calcite and vaterite obtained by precipitation, (Right)  $\text{CaCO}_3$ : pure calcite obtained by precipitation using a seed source (reproduced with the permission of Donnet et al., *Langmuir* 21 (2005); Copyright American Chemical Society).

Concerning the growth, there are several ways to control this step, by changing the solution composition-pH, conductivity, ionic species, impurities, etc., or adding organic species. Polymers can be chosen for their *specific adsorption* capacity on ceramic surfaces. These specific *interactions*, by inhibiting or promoting crystal growth in some directions, can change the final sizes and morphologies, or even block the precipitation. Precipitation is mainly controlled via the solid/liquid interface, but the chemist has to work out how to improve its control on materials properties by manipulating and understanding the processing parameters. Microfluidics and miniaturized systems allow a very fine tuning of the nucleation step, better exchange of heat and mass, while lowering heterogeneities in the reactor volume (Aimable in Llored *et al.*, 2013).

Chemists thus multiply the way selective relations are carried out. Nanochemists and materials chemists perform specific molecules or materials by means of asymmetrical dynamical relations located at different interfaces. In doing so, they learn how to control their synthesis using multifarious devices, chemical bodies, interfaces, and physical parameters. One should have chosen other examples such as: (1) combinatorial chemistry which produces ‘library’ of related chemical bodies by means of a systematic screening of potential curative substances; (2) sustainable chemistry which designs safer molecules and contrives new devices and methods in order to co-define their relative eco-toxicity—please refer to Sylvain Caillol, Olivier Godard, Isabelle Rico-Lattes and Laura Maxim’s papers within this volume; (3) chemical engineering which sets up new flow processes in order to achieve selective multi-step synthesis; and (4) ‘soft chemistry’ which uses weaker energy relations between ions, colloids, macromolecules, and clusters in order to synthesize ‘molecular templates’ situated in-between organic and



inorganic chemistry and which displays, for instance, catalytic properties. Those examples are as many relational strategies within which chemists produce and entangle heterogeneous chemical bodies while co-defining them by means of new relational classifications that fit environmental requirements (Llored, 2011, 2012a). Joachim Schummer asserts:

Chemistry at the core is a science of peculiar relations. Instead of studying isolated objects to be measured, compared and put into a classificatory scheme, dynamic relations between objects constitute the basic set of chemical knowledge, and, at the same time, provide the grounds for the classification of the objects themselves (Schummer, 1998, p. 131).

We would like to summarize essential points before moving to the second part of our paper. We have pointed out that chemical relations are pragmatically scrutinized within the context of a comparative chemistry. Analogy is the main guide followed by chemists to construe networks of independencies by means of chemical operations. The French chemist George Urbain asserted:

Each body being a collection of properties, the reasoning by means of analogy implies that those properties are not independent from one another. If one aims at facing the problem of analogy from a chemical standpoint, he/she must start querying under what limits those properties are interdependent (Urbain, 1921, cited in Bensaude-Vincent, 2008, p. 244, our translation).

Chemical bodies-molecules and materials-are defined by their selective capacity to interact with one another within a precise context and a particular field of practices. In this respect, action and relations seem prior to substances. But ‘it is only because our chemical species *per definition* retain their identity during purification, that we are able to connect single facts of chemical relations with each other to build a systematic network of chemical knowledge’ (Schummer, 1998). Pure substances are produced by one or different operations and chemists need them as ‘*relata* of chemical relations and, finally, as nodes of the chemical network’. Schummer adds:

The resulting classification has turned out to be again a network structure, with substance as nodes and chemical class relation as connections; it has enormous systematizing and predictive power with regard to chemical properties (Schummer, 1998, p. 157).

Relations allow chemists to define chemical entities and properties while operations allow them to obtain pure chemical bodies. Those bodies

then enter into new relations in order to obtain new compounds that, once purified, allow chemists to widen and to deepen their classification by analogy, and so on. The process is open-ended and depends on the modes of access –instrumental or cognitive. *Relata* are not prior to relations, and relations are not achievable without purifying operations and purified chemical bodies. *Relata* and relations are *constitutively co-defined*. They *co-emerge* within an *ordered and evolving network*. *Relata* are not independent from the relations but depend on selective operations or on chemical transformations. According to Bernal and Daza, chemical relations are ‘internal to the thing themselves’ in the sense that chemical properties and bodies are defined by means of selective relations (Bernal & Daza, 2010).

Chemical bodies are thus considered as instruments for action. In this respect, they release dispositions when interacting with other bodies or against instruments. Chemists ‘think with structural formulas’ and ‘work with’ chemical bodies to use Schummer’s turn of phrase. A chemist can interpret a structural formula in order to produce it from basic molecules—this strategy is called ‘retrosynthetic’ in organic chemistry—or to foresee its reactivity against other bodies. Structural formulas are thus ‘paper tools’ (Klein, 2003) which allow chemists to perform new reactions and which depend on a whole network of interrelated reactions and chemical bodies. In short, all those formulas, tables of rapports, periodic law, and nomenclatures are utterly relational in the same way as chemical bodies are defined by means of relations and operations. It is the reason why an epistemologist should move the instruments and experiments into the foreground of her epistemological work (Holmes, 1989; Holmes & Levere, 2000), if she aims at understanding how chemists co-define pure entities and chemical transformations from within their practices. Let us envisage a study led by Llored at the DCMR laboratory at the École Polytechnique–France—in 2010. It deals with how quantum chemists contrive and use their methods in order to explain and to foresee chemical reactivity.

### **Co-stabilization of Interrelated Chemical Practices: Back to the Laboratory**

Following Roald Hoffmann’s call for a ‘rotation laboratory’ (Hoffmann, 2007), we decided to explore quantum chemists at work (Llored, 2012b). We discussed with researchers and attended quantum calculations in order to understand better some steps that are not really present within scientific papers.

Kohn–Sham density functional theory-DFT-has become one of the most popular tools in electronic-structure theory due to its excellent performance-cost ratio as compared with correlated wave function theory, WFT. Within this theory, the molecular space is divided into grids of cubes; researchers define an electronic density for each point of this space. It is a holistic approach that enables quantum chemists to calculate molecular geometry or total energy exhaustively thanks to its electronic density—‘ $\rho(\mathbf{r})$ ’ under certain conditions. The total energy is in consequence a *functional* of the electronic density, that is to say a function the basic variable of which is the electronic density function (Kohn et al., 1996). Approximations are required because the exact electronic density cannot be reached.

This field of research aims at creating new density functionals with broader applicability to chemistry by including, for instance, non-covalent interactions. The crucial step is the *calibration* of new functionals against benchmark databases or best theoretical estimates (Goerigk & Grimme, 2010). The researchers of the laboratory DCMR explain to us that a best estimate is the best theoretical calculations available at the time of the calculation. This best estimate may be, directly or not, connected to an empirical value. The whole system consists of databases and best estimates which are stabilized at a particular time. The whole *network* is coherent; the results are highly *interconnected* and interdependent and depend on what chemists previously learn from their experiments and their chemical reactions.

Let us just take an example to figure out what is at stake in the device of basic functionals, which are tools that enable chemists to carry out their calculations. The most popular density functional, ‘B3LYP’, has some serious shortcomings among which is its underestimation of barrier heights by an average of 4.4 kcal/mol. This underestimation is usually ascribed to the self-interaction error-unphysical interaction of an electron with itself-in local DFT (Truhlar & Zhao, 2008). Moreover, B3LYP does not allow us to model transition metals satisfyingly and is totally inaccurate for interactions dominated by medium range correlation energy, such as Van der Waals attraction, aromatic-aromatic stacking, and alkane isomerization energies. So what do they do to improve a functional and thus to solve this problem?

Truhlar and Zhao change parameters and include new ones while shaping a new mathematical functional form that takes physical phenomena and chemical results into account. In so doing, they design a new functional by trial and error. They then use databases to appraise the reliability of a new functional within a defined purpose. The whole work is

pragmatic. As a matter of fact, two databases gather all the thermodynamic quantities: (1) the data base 'TC177' is a composite database consisting of 177 data for main-group thermochemistry including atomization energies, ionization potentials, electron affinities, proton affinities of conjugated polyenes, and hydrocarbon thermochemistry, among others data; (2) 'DBH76' is database of 76 diverse barrier heights concerning for instance nucleophilic substitution and hydrogen transfer. Truhlar and Zhao then *discuss the performance* of new functionals for these databases, they conclude that functionals labeled 'MO6-2X' and 'MO5-2X' are the '*best performers*' for the main-group thermochemistry and barrier heights. They propose cases study to exemplify their statement. The isomerization energy of octane involves stereoelectronic effects; none of the previous functionals gives the right sign for the isomerization energy from 2,2,3,3-tetramethylbutane to *n*-octane. The functional 'B3LYP' gives an error of 10 kcal/mol while 'M05-2X' *predicts* the right sign because this later allows a better description of medium-range XC energies, which are manifested here as attractive components of the non-covalent interaction of geminal methyl and methylene groups (Truhlar & Zhao, 2008). On the basis of 496 data in 32 databases, they *recommend* different 'best functionals' designed for transition metal thermochemistry, main-group thermochemistry, kinetics, and non-covalent interactions.

To sum-up, they change parameters before comparing their results to experiments or with best theoretical estimates. They compare the performance of a functional against previous ones and they then modify it again until a satisfying stabilization is reached. The three main words to describe this activity are: (1) pragmatism, (2) context-dependence, and (3) performativity. How do quantum chemists then choose one functional from another to carry out calculations?

The researchers from DCMR carried out a calculation in our presence. Choosing a functional of electron density depends upon: (1) the necessary accuracy, (2) the chemical system, and (3) the time needed for calculation. It also requires choosing a set of functions called a *basis* to achieve calculations for *each atom*. The basis changes according to the type of atoms, three main types are available depending on the situation to describe. They can also pragmatically use those three types within a linear combination according to the case. The basis also changes with other effects such as diffusion, polarization, pseudo potentials for core electrons, and the size of functions-double, triple zeta. All depends on circumstances. There is no generality within this work.

The functional and its relative basis set define a "level of calculation". The calculation process requires choosing a computer program such as

Gaussian type or Turbomole. An auto-coherent calculation can then start. Loops of calculations are carried out until the whole values reach a convergent minimum value. If calculations are not convergent, researchers can change the functional, the size of the grids, and convergence thresholds in order to optimize geometry or to calculate molecular energy. Each step reveals know-how, chemical culture, and pragmatic compromises.

Whatever the nature of the tools—molecular orbital, functional, and so on—may be, the calculation always uses both the *Variation Principle* to minimize the energy and the molecular structure which must have been determined by means of experiments. The variation principle is a technical device, which allows researchers to calculate the lowest average energy. Beyond its technical aspect, the very justification of this principle requires one to envisage *the relation of the whole molecule with its environments*—molecules, photons—in order to rationalize the whole process. This interaction with the environment may be explicit or implicit within the formalisms according to the case being studied. It depends on the situation. The interaction with the solvent may thus also modeled and sometimes taken into account. The very process of calculation thus holds together information about: (1) the whole system—its geometry that chemists first define from the outset of the calculation, (2) the parts—a functional for each atom or groups of nuclei, a molecular orbital, and so on, (3) and the solvent—what is outside the whole. The calculation uses the three levels—the molecular whole, its parts, and the environment called the solvent—*at the same time* in order to: (1) minimize energy, (2) calculate an energy barriers, (3) determining a transition state, and (4) for postulating a geometry by means of different levels of calculation, respectively.

The model of solvent is related to the solvation free energy of each compound. This quantity is always defined as the required amount of energy necessary to transfer a molecule of gaseous solute into the solvent. The crucial step is to appraise how the solvent gets involved in a chemical reaction. Its action can be direct if some molecules of solvent take part in the chemical process or indirect if the solvent—then labeled the ‘bulk medium’—only modifies reactants reactivity compared with that of the same molecules in the gas phase.

A particular level of calculation—functional and its basis—is only designed to reach a particular aim—final energy, geometry optimization, barrier height, and so on—and exclude the others. One cannot study all the molecular characteristics by means of a single level of calculation. When quantum chemists study the energy barrier of a chemical reaction, they have to choose a functional, its basis, and best estimates for each level—atoms, molecule, and the solvent. They thus tailor a useful tool to

understand and to predict a defined characteristic and not the other. ‘Complementary’ levels of calculation are thus necessary to achieve a global molecular description. Let us just quote a typical part of quantum paper to grasp the situation:

Calculations were performed with Gaussian 03. Geometry optimizations were conducted using the B3LYP method at the 6-31 G(d,p) level for the B, N, C, O, S, H atoms. The CRENBL relativistic effective core potential and the associated valence basis set were employed to model the iodine atom. This basis set is referred to as BS1. Each stationary point has been characterized with frequency analysis and shows the correct number of negative eigenvalues (0 for local minimum and one for a transition state). Energies were calculated for the stationary points at the B3LYP level using an extended basis labeled BS2. It consists in the 6-311+G(2d, 2p) for B, N, C, O, S, H, the extended Wachters basis [15s11p6d2f/10s7p4d2f] for Zn and the Aug-cc-pVTZ-PP basis set and pseudo-potential for I. We have demonstrated previously that this level of calculation gives reliable geometries and relative energies on zinc complexes (Picot, Ph.D. dissertation, chapter 5).

This typical calculation clearly illustrates what explaining a structure or a mechanism, and what predicting a transformation amount to. Quantum chemists use a lot of interrelated tools within a large and sophisticated network that *holds together* mathematical functions and devices, empirical outcomes, computer engineering, quantum and classical physics, and chemical knowledge and know-how. They tailor highly specific methods to account for chemical transformation. To do so, they use analogy between families of similar compounds. This work is utterly *relational*. Not only does it assemble multifarious tools within a coherent and performative practice of articulation but it also entangles the molecule, its parts, and its environment within the minimization of the total energy. Their method is *relative to* a family of chemical compounds and depends on the entanglement of inter-calibrated tools. Their method is *a way not the way to account for* a characteristic of the whole from its parts and its environment. In this respect, a quantum method is a practice of articulation that negotiates an explanation of the whole/parts relation. Isabelle Stengers asserts:

As soon as the question of emergence is at stake, the whole and its parts must thus co-define themselves, and mutually negotiate what an explanation

of the one from the others means (Stengers, 2003, p. 207)<sup>2</sup>.

In quantum chemistry, the mereology used by chemists entangles the whole, its parts, and, sometimes, its environment. It is not a classical transitive mereology in so far as the whole interacts with its environments. It is not merely a holistic description within which the whole is necessary to define the parts or the kinds of parts involved. It is not merely a classical mereology that only needs the parts to define a whole univocally. Quantum chemical practices need the whole, the parts, and the other entities at the same time, that is to say, a molecular structure, atoms or nuclei and electrons, and the solvent, respectively. Quantum methods are neither purely holistic nor purely reductionist. They always negotiate the articulation of different levels of description within a network that assembles chemistry, physics, computers, and mathematics. *Chemists have contrived specific methods within which the whole and its parts are constitutively co-defined* (Llored, 2010; Llored & Harré, forthcoming). Quantum calculations deal with types of patterns as possible values of contextual observables and not of monadic properties. Electrons, nuclei, atoms, groups of equivalent nuclei according to the NMR scale—an instrumental technique—or according to the group theory—a cognitive tool, basins or attractors from the theory of electronic density standpoint, are not intrinsic but are constituted by the modes of access involved. In this respect, they are relational and not monadic.

According to us, a new conceptual type of molecule is emerging. This new concept is the result of the *close interrelation* between technology and science. The *degree* of entanglements of a large variety of sophisticated quantum methods, mathematical tools, and computer devices with a large variety of new instruments, accurate captors, and metrological strategies has never been so strong. Molecule is now a “mixt” both of topology and experimental data. It holds together theoretical activities, modeling, and high-tech instruments in a novel and fine-grained manner. The novelty is that technology, science, and representation do not act independently from one to another. They are constitutively melded into a network of different practices. In what follows, we will refer to the following figure:

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<sup>2</sup> Our translation of the French sentence : “Dès qu’il est question d’émergence, le tout et les parties doivent donc s’entre-définir, négocier entre eux ce que signifie une explication de l’un par les autres”.

**The molecule is a unifying guide which holds together  
a network of open-ended practices**

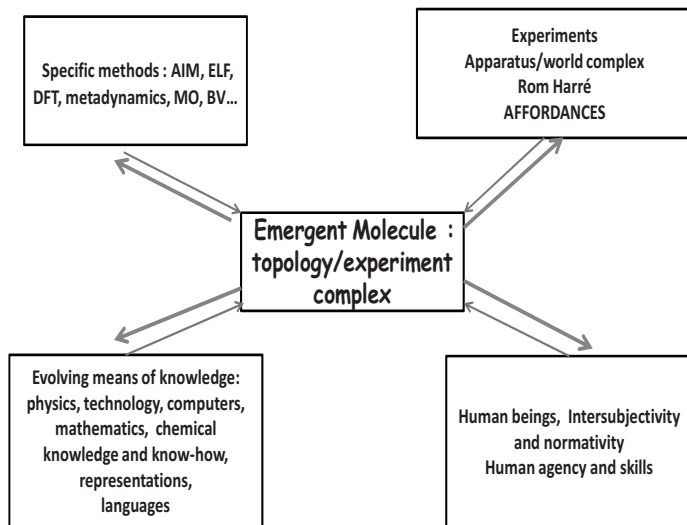


Figure 2: The emergent mixt kind of molecule (Llored, 2012b).

The emergent molecular conceptual scheme is highly technological and intertwines a large amount of empirical data and specific quantum parameters and integrals. This new molecular entity is defined by what we choose to call the “topology/experiment complex”. This molecule is *afforded* by: (1) specific and very often incompatible chemical quantum methods, (2) apparatus, (3) the articulation of heterogeneous means of knowledge, and (4) collective human skills, agency, and definition of normative rules. Feed-backs are manifolds in so far as this new kind of molecule also stirs up: (1) the design of new specific methods to determine a geometry or energy pathways, (2) the construction of new apparatus, (3) the emergence of new means of knowledge and practical know-how, and (4) the emergence of new skills, norms, and intersubjective agreements and projects. The emergent kind of molecule thus becomes a guide because it unifies without reducing multifarious practices within a network of relations. *The way chemists work is as relational as the chemical bodies they use by means of operations.* In this respect, chemical quantum practices as well as chemical entities are defined within a network of



relations. The close interrelation between technology, science, and human collective practices challenges the boundaries between theories and experiments, technology and science, philosophy of science and philosophy of technology (Llored, 2012b).

We have shown elsewhere that sustainable chemistry holds together multifarious practices entangled within a large variety of networks located at the interfaces between diverse scientific fields (Llored, 2011, 2012a). The reader can also refer to Caillol, Maxim and Rico-Lattes within this volume as regards sustainable chemistry. In the same vein, Ana Simões and Kostas Gavroglu make obvious that quantum chemistry is neither physics nor chemistry but a true novel specialty which intertwines chemistry, physics, pure and applied mathematics, and computer engineering. In this respect, the emergence of quantum chemistry is the convergent result of divergent scientific traditions (Simões & Gavroglu, 1997, 2011; Simões, 1993). The French historian of chemistry, Sacha Tomic, has cleverly shown that organic chemistry emerged from the interactions between analytical practices on mammals and vegetables developed by chemists and pharmacists during the nineteenth century (Tomic, 2010). Chemical practices often interlace a vast set of different know-how and knowledge. The mixture of practices and the transfers of concepts highlight the relational character of chemists' works. Following Rouse's discourse about the entanglement of practices while adapting it to chemistry, one could say: 'What results is not a systematic unification of the achievements of different scientific disciplines but a complex and partial overlap and interaction among the ways those disciplines develop over time' (Rouse, 1996, p. 135). At this step of our enquiry, we would like to query what kind of relational philosophy could be developed in order to meet chemical practices.

## **Towards a Relational Philosophy of Chemistry**

### **Dispositions and Affordances**

Several philosophers developed an ontology of *dispositions* adapted to chemistry. The status of dispositions may differ depending on the context. A chemical body can display a disposition *conditional on its being put* in a particular context. It can be 'acid' when opposed to water; it can become fluorescent when 'absorbing' a particular radiation, and so on. The idea of *intrinsic* dispositions is challenged by an epistemological approach within which dispositions are analyzed thanks to their *functional role* in scientific practices. From reified dispositions to functional ones, different philosophical

perspectives remain possible. As an example, Bensaude-Vincent focuses her work on what she calls “an operational realism” (Bensaude-Vincent, 2005, 2008; Bensaude-Vincent & Simon, 2008):

What we are trying to suggest here is that chemists’ practical philosophy is not limited to their notorious scepticism. The fact that they can marshal a population of material entities to perform useful work is itself a distinctive mark of chemists’ conceptual practices. For chemists, invisible entities are not primarily the keys for understanding the material world, the reality behind the phenomena, but rather a set of tools or instruments with which one can bring things about acting in the world (Bensaude-Vincent & Simons, 2008, p. 206).

Chemists *learn by making*. For them, “action comes first”. Following Ian Hacking’s ‘entity realism’ (Hacking, 1983) while reshaping Aristotle’s *dynamis*—meaning power or potential, Bensaude-Vincent proposes the denomination “operational realism” to account for chemical productive activity. Chemical bodies “exist” because chemists can do things with them. Including Nancy Cartwright’s account of capacities (Cartwright, 1989), Bensaude-Vincent and Simon add:

Limiting their ontology to agents that can act would be insufficient for chemists; they also need to postulate capacities for action (Bensaude-Vincent & Simon, 2008, p. 208).

Chemical bodies have dispositions to interact with other bodies in order to synthesize new bodies. Yet, dispositions or properties emerge through their mutual relations.

Rom Harré cogently calls for a return to instrumentation in order to grasp what scientists are doing. Following Wittgenstein’s approach, he scrutinizes practices and uses (Wittgenstein, 1953). He asserts: ‘Science is not only a cognitive enterprise but also a material practice!’ (Harré, 1986, p.281). Following Gibson’s work on the psychology of perception and Bohr’s complementary approach to quantum mechanics, Harré proposes the concept of *affordances* in order to make clear what scientists are studying with their apparatus.

The apparatus, its nature, and its way of working cannot be detached from physical phenomena. An electron-producing apparatus does not display particulate constituents of the atoms from which the electrons seem to come. Rather, it affords subatomic particles to the experimenter who is using the apparatus in a certain way. With a different apparatus, the experimenter can get the subatomic world to afford interference phenomena, with the same starting point as the experiment that afforded

particles. Harré asserts: ‘The way an activity is examined creates its distinctive picture, realizing certain affordances while excluding the manifestations of others’ (Harré, 2006, 501). It is a mistake to read back from products to constituents—atoms do not contain electrons as components, but they are such as to afford electrons given a suitable apparatus and suitable manipulations (Harré, 2013; Harré & Llored, 2013). ‘Affordances are a special kind of tendency, one for which the typical manifestation must be related to something specifically human’ (Harré, 1986, p.283). Three main categories of affordances can be singled out: (1) substantive affordances, for example, an alembic affording essential oils from raw plants; (2) affordances as attributes or properties—for example passing light through a prism affords a spectrum of colours. Without the prism or something comparable there is no spectrum. In this respect, specific lasers afford chemical fluorescence; (3) affordances as processes—for example, “ice-and-dog” afford walking but “ice-and-elephant” do not. Cloud chamber and electron source afford tracks, while collimator aperture and the same source afford interference rings. In this respect, flow process in chemical engineering affords a selective multi-step molecular assembly (Harré & Llored, 2013; Llored & Harré, forthcoming).

Harré introduces the key notion of “World/apparatus complex”: ‘But these dispositions are explained by reference to the causal powers of the world. How the causal powers of the World are manifested is relative to the apparatus or technique employed ... What has the power, the World or the apparatus/World complex? In dynamicist terms the World has the power, but while it is the apparatus/World complex that affords the display, that is to which dispositions are ascribed’ (Harré, 2004, p.205).

This *interfacial* concept enables Harré to question ontology by including both instrumental and practical standpoints. In so doing, he widens the scope and the depth of philosophical studies about science and even about humanity in general. Furthermore, he reflects upon some “mereological fallacies” committed both by philosophers and by scientists with regards to the conclusions that can be drawn from experiments such as chemical transformations and analysis. His work scrutinizes mereological strategies to understand the role of the part/whole relation in chemical discourses and in other scientific areas (Harré, 2013; Harré & Llored, 2011, 2013). Harré is fascinated by instruments, and the form of his practical philosophy queries human inventions, whatever their forms may be. His epistemology is based on a philosophy of *causal powers* that includes the different human forms of life, their open-ended hinges (Wittgenstein, 1979), the ‘World/apparatus complex’, and their articulation. Harré opens the way for another kind of epistemology that goes beyond

current philosophical dichotomies, such as the emergence/reduction debate by showing how to unify without reducing (Harré, 2006). Affordances are not intrinsic dispositions but the result of our interaction with the world. They also have a functional role of unification within the economy of knowledge and a heuristic power.

### **Towards a Pragmatic and Neo-Kantian Perspective**

Chemists define chemical properties by means of relations, say, by using chemical reactions. Pure compounds are obtained by operations of purification; they are not prior to human interventions. Chemical properties are co-defined by means of analogy and are constitutively dependant on modes of access—cognitive or instrumental. Tables of affinity, chemical formulas, and chemical classifications in general, are as many networks of interdependencies. Chemical *relata* and relations co-emerge within evolving practices.

Quantum chemists entangle the whole, its parts, and sometimes, explicitly or not, its environment within the calculations. They deal with types of patterns as possible values of contextual observables and not of monadic properties. Sustainable chemistry entangles reactional processes, chemical actors, and the environment at the same time in order to fit environmental norms. Sustainable chemistry is not a homogeneous community but encompasses multifarious ways of doing chemistry and chemical communities from nanochemistry to chemical engineering. Green chemistry is not a delineated field either. It does not have a pure and unique reference. A chemist who optimizes an extraction process using a supercritical fluid does not make use of the same practice of chemistry as a specialist of molecular assembly using transition metals. They are both chemists and mostly use the same molecular representations, but they do not have the same chemical culture and know-how. Moreover, they do not use the same resources in the same sites with the same aims: their scientific “forms of life” differ. A relational philosophy should thus scrutinize every chemical form of life in order to identify how chemists construe their networks of interrelated bodies.

Is disposition a *necessary* concept in order to make chemists’ relational strategies intelligible? Is an ontology of causal powers the only way to think about chemistry within an operative and practical framework? Is the new ontology of ‘active matters’—a new kind of pluralism about individuals endowed with capacities—the sole solution? We do not think so.

Ernst Cassirer, neo-Kantian philosopher of the Marburg school, asserted that the atom is never a starting postulate but rather a point of

arrival of the statements of the chemists. It is seemingly only that such or such property is then attached to the atom as with its “absolute support”, within a unit that appears to control and solidify the whole of the relation (Cassirer, 1910).

The atom is not a ‘thing’; it just makes it possible to federate knowledge (Llored, 2010). Cassirer pointed out that the positive benefit that chemical knowledge gains there consists in the systematic articulation of the ratios themselves. The initially dispersed facts start from now on to be organized; instead of coexisting in indifference, they are ordered around a center of precise reference. He upheld that the atom does not have for only logical value to provide afterwards for the description and the convergence of the recorded experiments. The unification thus construed plays an immediately productive role; it sets up a total diagram applicable to the future observations and assigns to them a given direction (Cassirer, 1910).

We could replace atom by molecule in this case, especially by the ‘topology/experiments’ molecule that we have previously defined. Chemists are often pragmatists about chemical bodies or entities. They use them to explain and to unify relational schemes without necessarily being realists as regards their ‘intrinsic’ existence—as it is the case for Mendeleev’s elements. In this respect, no intrinsic disposition is required to think about chemistry. At best functional dispositions could meet this unifying articulation of correlative chemical reactions, which only depend on operations and contexts. It is the reason why chemists always postulate a huge diversity of material entities—or abstract entities such as elements—within their practices. They are tools for doing further researches. Chemists need to act *as if* those entities existed while acting upon ‘them’. The way chemists are ‘realist’ is far more complex than the general philosophical meaning of the word ‘realist’ may suggest. They have their own pragmatic way to be realist!

Does one need to accept Hacking’s operative and technical criteria in order to define an entity as real? According to Hacking:

The entities of which we suppose reality must be capable of a causal effect on the real things took *prima facie*, i.e. over the material things of ordinary size. [...] We should count as real all that we can use to intervene in the world so as to affect something, or all that the world can use to affect us (Hacking, 1983, p. 242).

Actually, the change of status from hypothetical entities to real ones by means of action—chemical operations within our context—does not afford any ontological privilege to them. ‘Being real’ for an entity means ‘being

displaced' within the cognitive relation. As a matter of fact, the entities is first what is queried within a particular practice before becoming what is taken for granted to develop future researches (Bitbol, 2010, chapter 6). In this respect, putting this reality into question could cause a decrease in a collective efficiency within a research group. Far from leaving the cognitive relation aside as a provisional framework from which one could always take distance, assigning reality to a new kind of entity always amounts to reshaping the cognitive relation within a novel configuration (Bitbol, 2010, p. 404). Moreover, considering a disposition as a property means trying to capture the *idea* of a 'tendency to acquire' a property rather than claiming that the chemical body actually possesses this property. Asserting that a 'tendency' can 'cause' something to occur is a way of amplifying the previous mistake by reifying what is just an assumption which needs to be further elucidated (Bitbol, 2010, p. 124).

Chemical strategies entangle operations, formula, classification, and abstract entities in order to explain co-emergent entities and chemical reactions. Analytic and synthetic reasonings are intertwined (Llored & Harré, forthcoming). It is interesting to notice that chemistry and the kind of mereology related to it may help philosophers to redefine the frontier they drew between analytic discourse strategy and that of synthetic discourse and reasoning in so far as chemists are neither purely holistic nor purely analytic. In this respect, 'chemistry is very much a mixed science' to use Holmes and Levere's turn of phrase (Holmes & Levere, 2000, introduction, p. XV). Theoretical chemical approaches are neither ontic nor purely epistemic. They do not express exclusively the structure of reality out there, or the form of our own knowledge, but their *active interface*. We have previously illustrated this point when focusing on the pragmatism of chemists and the role of trial and error within the open-ended device of new functionals of density. Chemical mereology deals with this interaction between a whole, its parts, and the environment within chemists' work. Moreover, the whole is relative to its relation to other wholes within families of chemical compounds. Its acidity for instance is defined in comparison with other compounds. Its structure is relative to the solvent and can be studied by means of analytic methods such as NMR or radiocristallography of X-ray (Llored & Harré, forthcoming).

Chemical practices are constitutively mixed. Chemists always synthesize and analyze novel molecules or materials. We thus need a relational philosophy that simultaneously integrates the practice of networking interdependencies and the notion of emergence into its requisites. Pushing

this relational philosophy to its far end, we may reach the following radical conclusion:

*The world of physical phenomena is groundless throughout*<sup>3</sup>. This latter strong statement obviously does not mean that there *exists* nothing at all (which would be nihilism). Only that the overall process of which we partake by our action and cognitive relations has no fundamental level on which everything else rests. It has no absolute fundamental level and no absolute emergent level either, but it has co-emergent order. According to Wittgenstein's beautiful metaphor: 'One might almost say these foundation-walls are carried by the whole house' (Wittgenstein, 1974, 33<sup>e</sup>)" (Bitbol, 2007, p. 303).

Quantum chemical calculations exemplify this "co-emergent order" more clearly than any other science. All those mathematical tools, structural macroscopic characteristics, empirical data, and auto-coherent computational devices are co-dependently arising and are in turn connected similarly with other events or phenomena by means of finer-grained correlations. They all actively take part in the stabilization of a global techno-scientific network the cornerstone of which is the "topology/experiment complex" (Llored, 2012b). Electrons, nuclei, atoms, basins or attractors from the electronic density standpoint, are not intrinsic but are afforded by modes of access. In this respect, they are relational and not monadic. Parts, wholes, and local environments are constitutively dependent on the mode of access—instrumental or cognitive. In line with our former reasoning but extending it to chemistry and quantum chemistry, we consider that if the whole process is *groundless throughout*, then there may be emergence without emergent properties. Not asymmetric emergence of high-level properties out of basic properties, but *symmetrical co-emergence* of microscopic low-level features and high-level behavior. Not emergence of large-scale absolute properties out of small-scale absolute properties, but *co-relative* emergence of phenomena. Those phenomena, in turn, are to be construed as relative to a certain experimental context, with no possibility of separating them from this context. The notion of emergence thus gains credibility at the very same time it loses ontological content. In the same way, there may be inter-relatedness without efficient causality; and there may be upward *and* downward causation without *any* causal power. In a non-substantialist framework of thought, the issue of downward causation is not one of inherent powers, but one of relations and actions (Bitbol, 2007, 2010).

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<sup>3</sup> Michel Bitbol's emphasis.

A shift from Aristotle's efficient cause to an "interventionist" concept of cause is required within this context of relational emergence. Galileo Galilei asserted: "The cause is that which, when posited the effect follows, and when removed the effect is removed" (Galilei, 1612, 425). According to this perspective, if one intervenes at a higher level of organization, some effects of this action can then be detected by a mode of access specifically aimed at a lower level with the probability  $p$ . If the intervention is prevented, the former group of low-level phenomena vanishes (Bitbol, 2010, 2012). Whenever chemists change a solvent or whenever they transform the molecule by means of chemical operations at a coarse-grained scale, they can measure, for instance, changes in the emission of fluorescence or in bending vibrations at finer-grained scales. Whenever they change a "functional and/or its basis", say, whenever they change a level of calculation, to integrate a local diffusion, a polarization, or pseudopotentials for core electrons, among other microscopic effects, into the description, they can make the calculation converge at the molecular scale. Whenever this change is removed, the calculation keeps on diverging until chemists judiciously act by using the knowledge acquired from previous calculations, that is to say, by using a particular know-how. The former statement bearing on a pragmatic conception of downward causation is thus translatable into our context of quantum chemistry. Up to a certain point, it can also be adapted to the more general context of chemistry if one remembers that *relata* and relations are co-defined within chemical practices. In doing so, one should always bear in mind that chemists synthesize and analyze chemical bodies by means of operations within comparative taxonomies. Chemical compounds are always purified and then *categorized* by means of chemical reaction, that is to say, by means of relations. The relational work of chemists surprisingly needs not a substantialist framework of thought to be developed but merely a pragmatic use of networks of interdependencies. It is enough to know how to act selectively at one level, in order to modify what is measured at the other level. We can then add that in chemistry one is no longer concerned by issues about own-being but by interactive processes of which we partake by our instrumental and social actions. The scale of the object of interest is defined by the resolution of the tool that has been selected to manipulate it, not by any pre-existing elements that allegedly constitute either the object or the tool (Bitbol, 2007)

Modalities of action are of paramount importance within chemical works. Quantum calculations as well as chemical synthesis are indexed by a certain level of intervention-level of calculation, level of access, levels of actions, levels of theorization, levels of analysis. Emergence, downward



causation or upward causation should not be understood as substantial concepts, but rather as relational concepts throughout. Those relations contribute to the very definition of the terms involved within it. The quantum calculations contribute to the very *operational* definition of the whole, its parts, and the environment, just as the coupling between liquid chromatography and mass spectrometry contributes to the very determination of new thresholds that determine new norms and sustainable chemical designs. In this respect, emergent levels—molecules and materials from basic constituents, devices from norms, instruments from matter, ideas from within practices—are neither illusory nor real but *objective* in a pragmatist Neo-Kantian extent in so far as they are *constituted* inside evolving scales of intervention and modes of access. The co-emergence of levels or of chemical *relata* and relations are crucial within this perspective, which denies any ontological priority or ground.

To do so, two forms of allegedly incompatible epistemologies have to co-operate. Firstly, a naturalized relational epistemology which both aims at (i) scrutinizing the mutual compatibility between co-defined levels of organization, chemical bodies and reactions, and (ii) putting forward their dependence vis-à-vis means of knowledge—cognitive and instrumental. According to this approach, no reification of a level of description—atoms, molecules, coupled chemical reactions, chemical process, to quote but a few examples—is reached but only interrelations without prior ontological hierarchy. For example, this epistemology investigates how quantum chemists entangle the whole, its parts, and its environment within levels of calculations while using databases and best estimates. It also studies how quantum chemists articulate the result of incompatible methods to provide an overall molecular geometry, an energy surface, and information about transition states. It can also queries how chemists co-define eco-toxicity by means of analytical correlations or how they construe a ‘table des rapports’ or ‘a new periodic table’ by analogy.

Secondly, the former approach needs the support of a Neo-Kantian and pragmatic form of epistemology. This complementary epistemology studies the *evolving* and *functional* conditions of knowledge constitution, that is to say, the *practices* and the *forms of life*<sup>4</sup> belonging to a particular research field at a particular time. In doing so, a ‘rotation’ of attention to laboratory life is required in order to study chemical practices. This study pays attention to the conditions that make the identification of stabilized outcomes possible regarding a particular mode of intervention or of access. It aims at identifying co-defined configurations and relational

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<sup>4</sup> The word is to be understood in its Wittgensteinian extent.

invariants as guides for chemical actions, predictions, and explanations. For instance, it studies how the use of the variation principle allows the convergence of molecular descriptive parameters and thus an entanglement of different levels of organization by means of levels of calculation. It also scrutinizes the different ways of modeling depending on the research topic at stake in order to grasp how quantum chemists *functionally* and *pragmatically* account for their own practices. It highlights what temporarily allows quantum chemists to identify molecular invariants by putting into question the intersubjective modes of research tout court. It can also identify what are the constitutive assumptions that allow chemists to define and to refine the ‘Life Cycle Analysis’ used in order to design a novel molecule or a new sustainable process.

This cooperation between two forms of epistemology paves the way for interesting studies about the connection of philosophical concepts such as emergence with chemical or human practices while moving instrumentation, sites, and aims to the fore. As a matter of fact, it provides an open-ended unification of the various relations at stake without converging diverse perspectives into a unique and foundational one.

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# CHEMICAL ANALYSIS AS DEMATERIALIZATION

PIERRE LASZLO

## 1. Matter for chemistry

I wish to consider in this paper the relationship that chemists entertain nowadays with matter. I shall focus on its manifestations within the sub-discipline of chemical analysis, one of the goals of which is to make a formula correspond to a substance, whether unknown or to be identified. I shall first summarize laboratory practice: it will lead us to partial conclusions. I will present then a parallel with the study of language, which will lead us to a complementary set of conclusions.

Chemistry is routinely defined as the science of the transformations of matter. Does it mean that this science elects for consideration such or such a state, that it deals in particular with the various molecules that have been isolated or synthesized? In doing so, it would risk spreading itself too thinly. There have already been more than 66 million molecules collected in *Chemical Abstracts*. A regrouping into a much smaller number of classes is obviously necessary. In organic chemistry, for instance, such families can be organized with the help of *functions* (such as alcohols, acids, ethers, amides, etc.).

If chemistry then is not so much a science of the too diverse garments of matter, should it be considered instead as the study of their interconversions, *i.e.* of the reactions that atomic assemblies undergo from a given geometric configuration to another one? Not unlike the two sides of a coin, the two aspects do coexist. Chemical *statics* and chemical *dynamics* are these two complementary sides. Chemical science needs both. As we shall see, they share shoving aside the material basis of chemistry. This is their methodological demand. Such a move serves also as a generative *aporia*.

Let us consider the very first stage of chemical work, when it tackles a material sample in order to determine and to state its contents. The set of operations by which the number of compounds present in a sample and their identity are to be determined is termed 'chemical analysis'.

Let us give a concrete example. For this purpose, I turn to a newspaper article (Folléa 1997, p. 18). It is entitled "30, 000 contaminated teats withdrawn from sale" with the sub-title "A test in 'Que Choisir' has established the presence of carcinogenic agents". The body of the article has this sentence "their dosage draws upon highly sophisticated techniques of chemical measurement termed gas phase chromatography".

Contrary to the journalist's rhetoric, gas phase chromatography is a conceptually simple technique, as we shall see. Let us rather consider gas-phase chromatography as a prototypic example of analytical methods in the laboratory, today. We shall present it for its mission, namely to transform chemical matter into information. Thus, I shall try to make explicit what the journalist had found too elaborate for her own understanding (or for that of the readership of *Le Monde*?).

At the beginning, we have on hand teats for baby milk bottles, made of an elastic, plastic and smooth material, of a given color. In order to analyze this material, that presents itself as a solid sample, the very first gesture of the chemist is to transform it into a chemical sample: he needs to disperse, to separate from one another the corpuscles making up the bottle cap. For this purpose, the chemist dissolves a tiny fragment—less than a milligram will be more than enough—in a solvent, a liquid such as alcohol, ether or acetone (yes, the same kind as used to dissolve away nails). The ensuing solution contains henceforth, under the aspect of a seemingly homogeneous liquid, all the molecules that were present in the tiny sliver originally removed from the rubber teat. The conglomerate nature of the initial entities, as they existed in the material world of the teat, is already erased by this dissolving act.

The operator then injects with a syringe a fraction of this solution into an oven, in which the mix vaporizes. All the molecules, the solvent molecules and the dissolved molecules originally from the teat, are then carried along by a stream of an inert gas such as helium into a racecourse, strewn with obstacles. Molecules have to go through a long tube, whose length is of the order of a hundred feet, and that has been packed with grains of a polymeric resin, that slows down the gaseous flow. All the molecules that had been injected are borne on this gas flow and, in like manner as debris floating downstream in a torrent, they stick for a short or a long time to local obstacles, just as a tree log is more likely than a twig to be held up by a rock in the whitewater. Another analogy is that of a marathon in which runners would be confronted with obstacles, big and small, here a garbage can to skirt, there a boulder or a wall to climb, and so on.

At the end of such a course, molecules have been sorted out by their



size and polarity. Some have gone through faster. Others have been held up for a longer time. In short, a detector at the exit of the chromatographic tube records only, if separation was indeed efficient, homogeneous sub-populations: first the group of the fastest A molecules shows up; it is followed by less rapid B molecules; and so on, and so forth, till the slowest X, Y or Z molecules show up in turn.

That is the manner in which nitrosamines, most often as not quite toxic molecules, carcinogenic on laboratory animals, were shown to be present in the teats of baby milk bottles of the Rémond brand. It caused consternation and a degree of public worry: in the days following the first announcement, the manufacturer made an announcement answering the charges from the consumer organization (the "Que Choisir" people), the Secretary of State in charge of consumer items ordered some controls to be made, a ban was considered, etc.

But let us return to this workhorse technique of analytical chemistry, gas phase chromatography. It effected a separation amongst the molecules injected into the system, those from the solvent and those from the teat sample: it split an heterogeneous population into homogeneous groups, whose members were all identical in each of the resulting sub-sets.

The separation stage was followed by a detection stage: in one way or another, and let's not worry here about the make-up of the technical device used, the arrival of each pack or group of molecules at the end of their chromatographic marathon triggers an electric signal in a measuring apparatus. A material sample thus gets converted into information, in the form of a peak whose shape contains data, both about the number of molecules involved and about their type.

This is a process of *translation* and it is fundamental. Modern chemistry handles information as much as it handles material change. True, the latter constitutes the subject matter (a deliberate word-play). Nevertheless, as in the real-life case of the adulterated teats, chemists process almost from the outset a piece of information and work on various signals. These electrical ghosts stand for the real material samples. In the example at hand, chromatography, the chemist counts peaks on a screen or on a piece of recording paper (or has the computer make such a count), providing him with the number of different molecular species that coexisted in the original sample.

The next stage is to identify the present compounds. For this purpose, one resorts to a data bank or, alternatively, a technician injects known samples into the gas chromatograph, under identical conditions: when their peak superimposes with that of an unknown, an identification has been achieved. Even though this is no longer how one actually proceeds,

let us remember the principle.

And how does one actually proceed, nowadays? Each of the peaks is analyzed, one after the other. The attendant molecules are hit with a high-energy electron beam that breaks them and ionizes them into fragments. Those atomic assemblies thus bear a positive electrical charge, and a mass spectrometer weighs them according to their mass/charge ratio. Furthermore, the accuracy in the determination of their mass is such that one can determine the elemental composition of each of those ions from the known isotopic abundance for each of the elements (isotopes, let us remind the reader, are atoms sharing the same number of nuclear protons but differing in their numbers of nuclear neutrons). The principle remains the same as previously: attribution of an identity to a chemical species, a fragment from a molecule in the present case, from a 'signature' that unambiguously characterizes it.

Knowing that the molecular unknown, whose overall mass and thus elemental composition are already determined, includes a number of identified fragments, it is now possible to infer how these various component fragments are put together, just as working out a cardboard puzzle.

Mass spectrometry is a major resource in spectroscopic analysis. Another is nuclear magnetic resonance: absorption of electromagnetic waves, in the range of frequency modulation radio stations, by the magnetic moments of atomic nuclei, when the sample is immersed in a very strong magnetic field, provides a set of absorption peaks, termed a 'spectrum'. Each of the spectral peaks is a signature for a group of atoms that characterizes it usually unambiguously, such as a C=O carbonyl group, a CH<sub>3</sub> methyl group, or a C<sub>6</sub>H<sub>5</sub> phenyl group ...

## 2. The System of Signs

In doing so, the chemist has transformed-and I need to emphasize once again that the exact nature of the material devices ensuring such a transduction are of no import for this argument-the material system borrowed from nature into a set of signs and of representations, fit for both computation and sorting out by the brain. He may have resorted to, in complementary or independent manner to the methodology just described, combining chromatographic analysis with spectroscopic identification by mass spectrometry and nuclear magnetic resonance, determining the structure of an unknown molecule using X-ray diffraction on a crystal, provided that a crystal was available.

In any case, the result consists of a formula and of a three-dimensional

model, in which atoms are set according to their microscopic disposition. Their distances are represented on a proper scale. A glimpse shows atoms that stand as nearest neighbors, most of which are linked by chemical bonds. Just like a tax assessor considers a map of a piece of real estate established by a surveyor, or just as an architect looks at his (or her) construction to be on a dummy model, the chemist is able to examine on a molecular model in 'real' space the relations between atoms in a molecule, an entity otherwise so incredibly small that it escapes viewing, even to an instrument-aided eye.

The signalization inherent in the formula or in the model is to a large extent conventional, and it is for the time being the end result of an historical process, which had to a large extent already been completed by the beginning of the twentieth century. The main stages of this development can be identified as: the nomenclature put forward in the 1780s by Fourcroy, Guyton de Morveau and Lavoisier; atomic theory as introduced by John Dalton circa 1810; the notion, anti-positivistic but so masterfully productive, of *radicals* that we owe to Justus von Liebig, August Laurent and Jean-Baptiste Dumas around 1850;<sup>1</sup> and structural chemistry, started in the last third of the nineteenth century by August Kekulé, Archibald Couper, Jacobus Henricus van't Hoff, Achille Le Bel, Louis Pasteur and a few others.

Now to the components of this system of signs: these are the atoms from Dimitri Mendeleev's periodic table, together with the arbitrary typographical symbols that stand for them (C for carbon or Na for sodium) and together with, for each atom, the spatial configuration of the virtual bonds irradiating from it, and ready to link up with other atoms. For instance, there are three classes of carbon atoms, digonal, trigonal and tetrahedral, with two coaxial bonds, three coplanar bonds and four bonds directed to the corners of a tetrahedron, respectively. Thus described, these are idealized concepts, not unlike Platonic archetypes.

These elementary modules are then assembled together into molecules, according to a connectivity, provided by spectral analysis. For instance, the molecule of alcohol (= ethanol) consists of a methyl group (or radical)  $\text{CH}_3$ , linked to a methylene radical  $\text{CH}_2$ , that is linked in turn to an hydroxyl OH radical.

Let us remark, at this stage in our description, that chemical analysis has replaced those immediate phenomenological perceptions, an aspect, a

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<sup>1</sup> It is considerably more fruitful to think of, say the ethanol molecule  $\text{C}_2\text{H}_6\text{O}$  as the union between the two radicals, between the two fictitious species, ethyl  $\text{C}_2\text{H}_5$ , and hydroxy, OH, than to conceive of it as the adduct (which it is!) of the two very real and existing molecules ethylene  $\text{C}_2\text{H}_4$  and water  $\text{H}_2\text{O}$ .

color, a grain or texture, a smoothness or a shine in the light, of a material sample (a teat, say), by discrete microscopic beings, idealized, postulated, incapable of autonomous existence and perhaps also forbidden any real existence of a tetrahedral carbon or oxygen atom.

Let us also note the resemblance to features of language. The person I am talking with emits sound waves, whose amplitude and frequency vary over a fraction of a second. Nevertheless, I hear her say one of the phonemes from the English language, for instance that corresponding to the vowel in 'cut' which my ear has easily distinguished from the similar vowel in 'cat'. My brain has spontaneously performed a Fourier analysis; it has used a power spectrum that led me to identify the 'u' of 'cut'. This is a fertile analogy. One can push it quite far; radicals in molecules have an epistemological status resembling that of phonemes in speech utterances.

### 3. The Language of Spectroscopy

Let us work over this analogy a little more in depth. In order to identify nitrosamines in the teats of milk bottles for babies, first gas chromatography served to separate them from other molecules in the sample. In a subsequent stage, spectral analysis characterized those nitrosamines, providing a formula for each, together with the relative amounts.

Thus, spectral analysis acts like a language: it associates some signified, the formulas of the nitrosamines in this case, to the signifiers embodied by their spectra. Note that the true basic signifiers and signified are here, on one hand, the discrete absorption frequencies present in a spectrum, and, on the other hand, the groups of atoms, the radicals, present in a molecule.

Let me hasten to point out the difference to a natural language: In spectral analysis we are not dealing with an arbitrary coupling between the sign and whatever is being signified. To the contrary, there is an intrinsic basis for such an association, both empirical and necessary: a given peak, at a certain frequency and of a certain shape, in the NMR spectrum of ethanol signifies methyl, not because I want it to be so, but because it is indeed so. The only arbitrary aspect, here, is denomination, *i.e.* use of the term 'methyl' for this  $\text{CH}_3$  group of atoms.

It is important to the present argument that spectral analysis—to which I shall give, without necessity for further justification, the role of an allegory for chemical analysis, taken more generally—has replaced matter by a spectrum (or by a set of spectra). It will rest its further logic on those ghosts exclusively. These ghosts have become the only reality. Henceforth, the original material, or matter, will remain shelved.

At this stage in his work, the chemist holds the spectrum as the only reality. The spectrum stands as the trusted representative of a molecular population, otherwise imperceptible to our sensory organs. The chemist reads the spectrum as an ordered set of signs that points to a given type of molecule or macromolecule from the material sample.

However, the spectrum, rather than an end in itself, is a mere stage in a process. As soon as it has been read and understood, a molecular object is unveiled behind or underneath it; and in turn it pushes away the spectrum. And this molecular object assumes the shape of one or another representation-in itself arbitrary: one can represent ethanol in dozens of different ways, as a set of touching spheres, or as interpenetrating balls, or yet again as sticks and balls -, which in itself serves as the form that a protean reality temporarily assumes for the chemist. The various models of molecules in the chemical imagination constitute languages akin to the other languages that humans resort to. Chemists agree as to their lexicon and to their construction or syntax, and they are well aware of their conventional nature.

#### **4. Mutation of the Laboratory: From Work on Matter to Transformations on Signs**

Thus the laboratory finishes being the locus for a symbolical work on matter. True, chemists continue performing actual material operations on substances. Besides the most important, their synthesis, they also do their isolation, purification, or yet various modifications aiming at improving, say crystallization, or, in another sphere, that of biological activity, the ability to serve as an efficient drug.

By then, the dematerialized work, if it does not subsume yet the material work, this intellectualized part of the chemists' task has already equal status. Its main tool is at present the computer: to help representing molecular objects by three-dimensional models; to predict vibrational frequencies in the infrared; to predict in like manner the aspects of nuclear magnetic resonance spectra ( $^1\text{H}$  and  $^{13}\text{C}$ , foremost); to map out the electronic density or the electrostatic field at various points in space, relative to the positions of the nuclei in a molecule; to likewise guess the wavelengths of the absorption maxima of visible light and thus predict the color of a molecule; and so on, and so forth.

Going from the macroscopic scale, that of the sensory, to the microscopic scale, that of the postulated molecular object, via the intervening molecular assemblies, is accompanied with another mutation, from experimental observation to theoretical calculations. The goal of

chemical analysis, nowadays, might be defined as the alphanumeric listing of the components in a mixture, in any mixture.

For this purpose, the perspective on matter has become demographic. Any sample is considered as a set, with various sub-sets or sub-populations, comprising a number of molecular individuals. These are determined at an astounding level of precision and accuracy.

The history of chemical analysis, that of the discovery (by Bunsen and Kirchhoff) and of the rise of spectroscopy, can be read thus both as a history of the progressive rise in sensitivity of measurement and as a history of the gradual distancing from reality: it has jettisoned the immediate properties in favor of the mediated properties.

When in the eighteenth century Gabriel Venel wrote the *chemistry* entry for the *Encyclopédie*, two kinds of analysis were being performed, analysis by fire, and analysis by menstrues (*i.e.* by what we now term 'solvents'). These two analytical modes have given rise to spectral analysis, and to chromatographic analysis, respectively; but at a cost, that of a removal.

Take the case of chromatography: in between the chromatogram and the material sample that it represents, at first stands a solvent; then, a black box filled with grains made of various resins, the 'support'; followed by another solvent or eluent, whose role is to sweep the molecules adsorbed on the chromatographic support; then one finds a detecting device (measuring, for instance, changes in the refractive index); a converter producing an electrical current, leading into another black box, packed with electronic instrumentation and digitizers: signal amplifiers, adding machines, data-smoothing and -integrating devices and software, etc.

To give a full picture, as a rule samples have become minuscule, in amounts generally between micrograms and milligrams. One may safely conclude that present-day chemists 'handle' mostly mental representations. The chemical laboratory, more than the site of transformations of matter, has become predominantly a production center for concepts.

## **5. Should Chemical Synthesis be Held as a Rematerialization?**

It is customary to pit analysis and synthesis as the two sides of a coin, as activities complementary to one another and to some extent symmetrical. The former clearly enjoys historical priority. The latter can be dated, referring only to milestones, to Wöhler's synthesis of urea in 1828, with the subsequent anti-vitalism slant that was given to it, and to

the syntheses by Berthelot of prototypic molecules such as acetylene and benzene during the second half of the nineteenth century.

The above description of analysis as a process of dematerialization might lead the reader to expect, as a contrast and by way of a satisfactory and expected resolution at the end of this paper, a presentation of synthesis as the indispensable rematerialization; which, of course, is true to some extent, but only in a rather naive and superficial approach. Each of the steps in the multi-stage synthesis of a complex natural product, such as those of quinine, strychnine or taxol, translates into access to an intermediate that can be weighed and identified through its spectroscopic analytical data, in the manner of a newborn.

However, the reality of the synthetic effort is elsewhere. It is an algorithmic process, it is a logical concatenation (computer-assisted too) in which radicals are gradually added to a structure, to that particular molecular architecture being erected. In synthesis, just as in analysis, idealities are dominant and they rule over any materiality. Matter dares to show up only at the very end, when the overall yield (or that for an individual step) is determined.

The reader may protest: is there no return to reality, to this proto-form matter, sometimes lumpy, sometimes fluid, that can take up so many incredibly diverse and unpredictable aspects, and which is to be found contained by and in the glassware that chemists handle in their laboratories?

The answer not only is "yes", it is also an interesting one! The molecular object, this representative of the molecule in the form of variously colored balls (atoms) connected by sticks (bonds), this molecular model that the chemist holds in his hands, or that he examines on the screen of his computer terminal, has the function for today's chemists of a kind of *substitutional hardware*. The molecular object is thus a close parent to the transitional object, *as defined by psychoanalysts such as D.W. Winnicott*.

Another easy and obvious temptation should be mentioned: to seek a rematerialization in chemical industry, since chemical science in academic laboratory seems to have jettisoned the materiality of chemistry. This ploy won't work though! In spite of chemical industry harboring some of the high temples of empiricism, any visitor of a chemical plant becomes quickly aware that the only matter he will see is either some of the primary material or some of the finished and packed product. The rest remains invisible; it is the province of chemical engineers who stand close guard over transfers of heat and material through large pipes.

The reactors proper, the interconnecting ducts with the occasional outlet of water vapor fumes, are all controlled from a set of terminals and

gauges for pressures, temperatures, viscosities, etc. at various locations in the huge network: matter has been screened off from the viewer by a complex hydrography, monitored and directed via computers.

Thus, we are led to the conclusion that chemistry is a science of matter in a formal sense only. It is, to a much greater extent, a science of mind. Like music, chemistry is a combinatorial art and science. In the same way as music goes beyond acoustics, chemistry transcends matter and has the intellect as its dwelling place.

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# A PRAGMATIC APPROACH TO THE ATOMIC MODEL IN CHEMISTRY

MANUEL BÄCHTOLD

Initiated in the late 19th century by Peirce, pragmatism in philosophy was developed and made famous in the early 20th century by James and later by Dewey. It experienced a new surge of success in the field of epistemology during the second half of the 20th century, under the impetus of influential authors like Rorty, Habermas, Putnam, and Brandom. In substance, pragmatism conceives of knowledge not as a frozen and preexisting entity that scientific research strives to discover, but as the ever-changing product of our adaptation to the world. The question this philosophical approach attempts to answer is not “What is the world like according to accepted theories?” but rather “How were the theories constructed and how are they used in scientific practices?”, where the term “practices” refers here to both the theoretical and experimental work.

The pragmatic approach seems to find a particularly relevant field of application in the epistemology of chemistry, a science where the manipulations of researchers and their observable effects play a major role in knowledge construction and use. Several authors in this domain, including Nye (1993), Psarros (1998), Schummer (1998, 2006), Zeidler (2000), Bensaude-Vincent (2003), Bensaude-Vincent & Simon (2008), Bernal & Dazal (2010), Llored (2010) and Harré & Llored (2011), have pointed out aspects of chemistry — both in how it is structured and how it works — that are echoed in pragmatic thinking.

The purpose of the present article is to sketch out a possible way of implementing pragmatism in the epistemology of chemistry. With the atomic model at the heart of discussions about what chemistry is, or at least about whether or not it can be reduced to physics, I propose to focus here on the use of the atomic model in this science.

## **1. The Atomic Model in Chemistry: A Historical Perspective**

### **1.1. The Atomic Model as the Cornerstone of Chemistry?**

What role does the atomic model play in the theoretical framework of chemistry? According to physical chemistry textbooks, which represent the most widely accepted ways of thinking (or at least in the area of university teaching), the atomic model provides the building blocks of this science. The textbooks very often begin their description of chemistry with a chapter on the atomic composition of matter. For instance, the well-known American textbook written by Atkins (2010), *Physical Chemistry*, begins with a chapter entitled «Fundamentals» describing matter as consisting of atoms. Similarly, the textbook of Lawrence, Rodger & Compton (1996), *Foundations of physical chemistry*, which provides a concise presentation of physical chemistry, begins with a chapter called “Atoms and ions: the building blocks of all matter” (p. 1). By placing the atomic model in first place in the description of physical chemistry, these textbooks convey the idea that this model constitutes the theoretical foundation of this science.

At first glance, this idea seems self-evident. It can nevertheless be qualified in the light of the history of chemistry since the early 19th century when Dalton explicitly introduced the atomic model into chemistry. In the course of the 19th century, the atomic model — which was still in a rudimentary form that could be summarized in terms of indivisible chemical entities combinable in multiple ways — was a useful theoretical instrument that accompanied rather than founded the theoretical work of chemists. In the 20th century, this early model underwent some theoretical developments and it was the version proposed in quantum mechanics that took its place (the latter describes the atom as being composed of a nucleus and electrons, entities endowed with a complex and powerful mathematical formalism). However, physical chemistry, which extended the quantum model to the molecular level, did not appear as a strict derivation of quantum theory but as a hybrid product associating the quantum model of the atom, to empirical knowledge of laboratory chemistry. Let me develop these two points.

### **1.2. The Atom in 19th Century Chemistry**

It is true that many 19th century chemists considered the atomist hypothesis to be very fruitful, i.e., useful for treating many chemistry

problems, but they still had reservations about the ontological question of the atomic composition of matter. They were either skeptical about it, or they saw the question as being beyond the scope of chemistry. For instance Kekulé (1867, quoted by Bensaude-Vincent, 2003, pp. 183-184) wrote:

The question whether atoms exist or not has but little significance from a chemical point of view: its discussion rather belongs to metaphysics. [...] I have no hesitation in saying that, from a philosophical point of view, I do not believe in the actual existence of atoms, taking the word in its literal signification of indivisible particles. [...] As a chemist, however, I regard the assumption of atoms, not only advisable, but absolutely necessary in chemistry.

On one side, all chemists used the atomic model in their research. As Rocke (1984, p. xiii) emphasises: “In terms of practice—and ignoring rhetoric—virtually all chemists after Dalton were chemical atomists.” On the other, the belief in the existence of atoms, at the ontological level, remained a question of personal choice and was not consisted a concern of science *per se*. As Knight (1992, p. 120) puts it: “Chemists [...] recognized atomism as a kind of optional extra.”

Based on the experimental data obtained in chemistry, it was not possible to directly infer that atoms existed (as Laurent thought<sup>1</sup>). As the 19th century progressed, however, the atomic model became increasingly useful in the chemists’ work, to the point of becoming inescapable. Knight (1992, p. 124) points out that in the 1860’s, “the deductive power of the atomic theory was becoming evident [...] the atomic theory now enables definite predictions and detailed explanations to be made.”

Historical studies converge on this point. The most important thing for chemists in doing their research was to dispose of the theoretical tools that enabled them to describe and predict the properties of chemical substances and their reactions with each other (see section 2.4). And the model of the atom was precisely such a tool. This point is expressed by Schütt (2003, p. 239) as follows:

The aim of the nineteenth-century chemists was not to explain matter and affinity *per se* but to forge theoretical tools in order to arrange the many empirical data coming out of the laboratory in such a way as to explain both chemical behaviour of known substances and predict new substances.

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<sup>1</sup> See on this point Knight (1992, p. 121).

In other words, the goal of chemists was not to describe the fundamental structure of the physico-chemical world, but to describe and predict chemical phenomena observed in the laboratory. This is supported for instance by Bensaude-Vincent & Simon (2008, p. 185):

Dalton's atom was intended to account for the discontinuity in combining proportions observed in chemical reactions, and not to provide a theory concerning the structure of matter.

Although referring to atoms turned out to be very useful in the practices of chemists, it was perhaps not as necessary as Berzelius claimed (see the above quotation). At least that is what Chalmers (2008, p. 160) contended in saying that the symbols introduced by Berzelius—and employed today to stand for the chemical elements—was only used by 19th century chemists to refer to masses and volumes:

The symbols in formulae [introduced in chemistry by Berzelius] do not have to be interpreted as referring to atoms. Any portion of hydrogen whatsoever can be chosen as the standard and the 'atomic weight' of another element determined in terms of the weight of that element that combines with the reference portion of hydrogen. It is this latter interpretation that accords best with how chemists determined relative atomic weight in the laboratory. They worked with weights and volumes rather than atoms.

### **1.3. The Atomic Model in the Development of Quantum Chemistry**

Following the experiments conducted in the late 19th/ early 20th centuries, which received a simple and convincing interpretation in terms of atoms and their constituents (especially those of Becquerel in 1896, Thomson in 1897, Rutherford in 1911 and Perrin in 1912), as well as the advent of quantum mechanics in 1925-1926, the atomic model finally became mandatory in physics and chemistry, and more specifically, the quantum-theory version. Many scientists then hoped to reduce the description of the properties of chemical substances to this theory. Quantum chemistry, i.e., quantum mechanics applied to the molecules of chemistry, developed thanks to the decisive contributions of Pauling and then Mulliken. Several new theoretical bases deemed fundamental were brought from quantum mechanics into physical chemistry, notably the notion of electron spin for understanding covalent bonding between atoms, and wave functions for predicting certain properties of molecules such as electron energy levels.

At the present time, however, chemistry knowledge has not yet been fully reduced to the atomic model of quantum mechanics. Is there some practical problem that needs to be solved or is a complete reduction impossible in principle? This question still divides the community of chemists. At the practical level of mathematical calculation, it proves very difficult to find stationary solutions to Schrödinger's equation in order to make predictions about complex systems like molecules. Granted, since the 1960's computers have been offering powerful tools for making such calculations (see for example Dykstra *et al.*, 2005), but finding a strict solution to Schrödinger's equation for multiple-electron systems is still not feasible. Two procedures for finding solutions are currently being used. The first involves simplifications or approximations. For example, in the LCAO method (linear combination of atomic orbitals), the wave function (which in theory should be associated with a system composed of several electrons) is replaced by a linear combination of wave functions each associated with one electron taken individually. Other approximations can be made, such as considering only valence electrons or ignoring the repulsive force of electrons. The second procedure consists of replacing theoretical terms that are difficult to calculate by data obtained experimentally (using various spectroscopic techniques, for example). When the first procedure is utilized alone, we speak of "*ab initio* methods"; when the two are used jointly, we speak of "semi-empirical methods". The first type of method finds solutions for small or medium-size molecules, whereas for large molecules, semi-empirical methods are generally employed (on this point, see for instance Thiel, 2005). In short, based solely on the equations of quantum mechanics, it is impossible in practice to directly infer and assign quantified properties to chemistry's molecules.

In addition, not all chemical properties can be inferred from approximations and/or empirical data. According to Scerri (2007, p. 924):

In the case of elements we can predict particular properties perhaps such as ionization energies but not chemical behaviour. In the case of compounds, what can be achieved is an accurate estimate, and in many cases even predictions, regarding specific properties in compounds that are known to have formed between the elements in question. Quantum mechanics cannot yet predict what compounds will actually form.

In its current state, then, quantum chemistry does not satisfy a major theoretical expectation of chemists, namely, predict what molecules, and thus what chemical substances, will be formed. However, chemists very

often call upon it to model the mechanism underlying a given chemical reaction.

Beyond this limitation of a practical nature, the possibility of completely reducing chemistry to quantum mechanics is debatable. Clearly, the conceptual framework of the quantum theory of the atom must be expanded before it can be extended to molecules and provide explanations of chemical properties and reactions. A case in point is the work by Mulliken: this chemist had to develop several new concepts in order to conduct his theoretical work in quantum chemistry, as those of “molecular orbital” or “bonding power” (on this point, see Llored, 2010).

The molecule lies one complexity level above that of the atom. Yet going from a single isolated molecule to a chemical substance composed of a great number of molecules represents a much bigger jump in terms of complexity. Doing so involves new properties (such as acidity or solubility), and describing these properties requires new theoretical and conceptual tools that are not yet part of quantum theory. For this reason, certain authors contend that reducing chemistry to physics is no more than a “myth” (Liegener et Del Re, 1987).

The debate about reducing chemistry to the quantum theory is certainly still open, but it has become clear that current knowledge in chemistry was not derived directly from the quantum theory of the atom. Granted, this theory produced invaluable new theoretical tools for developing physical chemistry. But the theoretical framework of quantum chemistry seems sightless without the experimental knowledge of chemical substances that chemists have been accumulating for over two centuries, and without the models and classification systems developed on the basis of that experimental knowledge. This point is made by several historians of chemistry. Nye (1993, p. 277) for example argues that “quantum wave mechanics gave chemistry a new ‘understanding’, but it was an understanding absolutely dependent on purely chemical facts already known.” Simões (2003, p. 404) also stresses that although quantum chemistry could not have developed without the theoretical tools provided by physics (or more exactly, by quantum mechanics), it was “guided” by knowledge of “empirical chemical facts”. Bensauade-Vincent & Stengers (1996, p. 243) draw the conclusion:

‘Quantum chemistry of the elements’ was therefore not deduced from quantum mechanics but rather reconstructed from disparate elements, some from quantum mechanics and others from data theorized by chemistry.

Given this historical perspective, it seems important to alter the image that physical chemistry textbooks present of the atomic model’s role in the

theoretical framework of chemistry. Today's physical chemistry is not derived from the atomic model of quantum mechanics, but is rather the merged outcome of the atomic model on the one hand and empirical knowledge established in laboratory chemistry on the other.

## 2. Why do Chemists use the Atomic Model?

### 2.1. Matter is made up of Atoms: A Not-so-obvious Ontological Assumption

Why do chemists use the atomic model? The answer seems evident: because matter *really is* made up of atoms, or stated differently, because this model describes reality as it is. This ontological assumption is found in a good number of physical chemistry textbooks. For example, Atkins (2010, pp. 1-2) writes: "Matter consists of atoms. [...] A chemical bond is the link between atoms. [...] Bulk matter consists of large numbers of atoms, molecules, or ions." Not only do these textbooks begin with a description of the atomic model, which conveys the idea that it is the basis of physical chemistry, but they also explicitly state that matter is composed of atoms. In other words, they jointly support two assumptions: that physical-chemistry knowledge can be "theoretically" (or "epistemically") reduced to the atomic model, and that matter can be "ontologically" (or "constitutively"<sup>2</sup>) reduced to atoms.

There is no logical implication between these two assumptions, for they are to some degree independent of each other. The fact that, today, chemistry has not been reduced to the atomic model (of quantum mechanics) does not refute the assumption of ontological reduction. It is fully possible to contend that matter is composed of atoms, or more specifically, that the observable properties of matter are due to physical processes involving atoms, irrespective of the extent to which such a reduction has been achieved at the theoretical level. This is for example the view supported by Le Poidevin (2005, p. 120): "there is, I think, a strong intuition that ontological reduction is true, whatever the fortunes of epistemological reduction."<sup>3</sup> Nonetheless, ontological reductionism can be called upon to justify the theoretical reduction: if matter is composed of atoms, it is legitimate to ground chemistry (or at least, to attempt to do so) on the atomic model. This line of reasoning amounts to saying that if

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<sup>2</sup> Concerning the terms "theoretical", "epistemic", "ontological", and "constitutive" reduction and their definitions, see Sarkar (1992) and Brigandt & Love (2008).

<sup>3</sup> The arguments of Le Poidevin are discussed by Scerri (2007).

chemists want to describe chemical substances as they really are, then they have to describe them in terms of atoms.

Although widely accepted, the ontological assumption that matter is *really* composed of atoms is not obvious. In epistemology, one can find arguments for it, supplied by "scientific realism", and arguments against it, those of "anti-realists". Undoubtedly the strongest argument in its favor is the "coincidence" argument (Hacking, 1983, Cartwright, 1983, Psillos, 1999), which goes as follows: the fact that there are very many experiments that can be satisfactorily interpreted in terms of atoms, cannot be a coincidence and shows that atoms really do exist.

There are at least two counter-arguments refuting the coincidence argument. The first is the so-called "circularity argument" (Putnam, 1981, 1995). Although Putnam did not forward this argument to respond specifically to the coincidence argument, it can be reformulated as follows: the fact that we find the manifestation of atoms or their properties in a large number of experiments is not surprising and is indeed not a coincidence, because what we are finding in each of these experiments is simply the entities we introduced in our initial description of the world.

This argument is not crippling for scientific realism. It is possible to reply to it as follows: the fact that our description of the world in terms of atoms applies in a satisfactory way to a very large number of experiments shows that this description is correct, i.e., atoms really exist.

The second argument against the ontological assumption about the atomic makeup of matter, surely the strongest (and the most highly debated), is the "underdetermination of the theory by experiment" (Duhem, 2003 [1908], Quine, 1975, van Fraassen, 1980): in principle, there are always several competing theories capable of describing the same set of experimental data (argument potentially founded on Duhem-Quine holism, according to which a theory's hypotheses cannot be tested by a single experiment but only collectively). It follows that it is not legitimate to state that a theory is true because it is empirically adequate.

This is not a mere argument of principle. It can be clearly illustrated in the case of interest to us here, quantum mechanics. Quantum mechanics has a rival theory, Bohmian mechanics, which is capable of generating all of the former's predictions and therefore has the same degree of empirical validity (see Cushing, 1994, Chap. 11). It is true that, like quantum mechanics, Bohmian mechanics rests on the atom hypothesis, although it doesn't offer the same model. One important difference is that in Bohmian mechanics, any physical system (e.g., an electron, an atom, or a system with more dimensions) is described as having an intrinsic position that is well defined at each instant and evolves in a predetermined manner. In the



case of quantum mechanics, the position of a physical system is generally not well defined, and the outcome of a measurement of it usually cannot be predicted. As a consequence, even if we had some indisputable means of justifying the assumption that atoms exist (which we don't), the fact remains that experimentation underdetermines the model that describes those atoms.

Coming back to the initial question: "Why do chemists use the atomic model?" According to the argument whereby the theory is underdetermined by experiment, the most obvious answer — "because this model describes matter as it really is" — is not receivable: not only are experiments unable to prove that atoms exist, they also do not determine unequivocally how atoms should be modeled. If we take this argument seriously, we need to look for another answer.

## 2.2. "Methodological Culturalism" in Chemistry

An alternative answer was proposed by Psarros (1998). According to this author, chemists' recourse to the atomic model can be explained by the "semantic function", which the terms describing atoms and molecules fulfill. Before looking more closely at this idea, let me briefly describe the framework in which it has been defended.

Psarros distinguished two approaches that emerged from the analytical tradition in the philosophy of science: the "naturalist" approach, which he uses to criticize, and the "culturalist" approach that he advocates (*Ibid*, p. 186). The naturalist approach sees science as the "sole authority" for assessing the legitimacy of a theory and judging whether the entities it postulates (such as atoms) really exist. Psarros noted that this idea contains "fallacious" reasoning. Indeed, the history of science and scientific methods is contingent, in such a way that the latter can only play a "normative" role. He argues (*Ibid*, p. 187):

There is no reason that forces us to accept a given description of a scientific method as compulsory for other scientific enterprises. Further, since the entities—corpuscles, forces, fields etc.—that occur in scientific theories have been introduced in order to explain phenomena that had been observed and reproduced *before* the invention of those concepts, it is a *petitio principii* to regard the same phenomena as a proof of the literal existence of these entities.

This means one cannot say, on the basis of the current scientific methods, if a theory is the good one and/or the entities it posits really exist.

According to Psarros, the default of the naturalist approach, responsible for the logical failure, is to ignore the cultural context within which the theories are rising. If he advocates for the culturalist approach, it is precisely because it takes account of this cultural dimension: “The culturalist approach regards science as a man-made process serving the achievement of aims that are formulated in cultural contexts” (*Ibid*, p. 189).

The “problem” this approach has to solve is the following: what warrants that the meaning of the scientific terms can be “transsubjectively” and “transculturally” communicated (*idem*)? In Psarros’s view, the warranty can be found in the everyday life “practices”, which are reachable to everyone irrespective of her/his scientific knowledge

Without being explicit, Psarros suggests that this transsubjective and transcultural agreement on the meaning of the scientific terms in chemistry does not exist yet. To enable this agreement, he proposes to reconstruct “methodologically” the vocabulary of chemistry by referring it to the “actions” that everyone can reproduce. These actions are associated to basic practices (such as metallurgy, tannery or pharmacopoeia), which are progressively enriched with the contribution of chemistry. The reconstruction of the vocabulary of chemistry amounts to determine the semantic function of the chemical terms in the frame of these practices and to redefine them.

Psarros makes the distinction between several kinds of functions. For instance, terms like “measurement” or “x-ray spectrometer” have a semantic function of “predicators”, i.e., they enable to “distinguish and to describe actions, things, situations and processes” (*Ibid*, p. 194). In regard to the terms describing atoms and molecules, Psarros supports they have a “the semantic function of *theoretical terms* or *theoretical concepts*” (*Ibid*, p. 197). What does it mean? Psarros is not that clear on this point and answers with an example, namely the one of the experimental law of Gay-Lussac stated in 1808 (according to which the ratios between the volumes of two reacting gases are ratios of small integers): the function of the terms describing the properties of atoms and molecules are to “explain” this experimental law.<sup>4</sup>

Psarros not only tries to determine the semantic function of these terms, he also claims that atoms and molecules do not exist outside the scientific theories: “Molecules occur only in scientific theories. Therefore we will call such an entity a *theoretical construct*.” (*Ibid*, p. 197).

The merit of the culturalist approach is that it brings out how chemistry is rooted in practices. However, it can be criticized on several accounts.

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<sup>4</sup> Psarros does not tell us what his conception of an “explanation” is and if the latter is different or not from a classical one.

Firstly, doesn't the description of actions as the building blocks upon which Psarros plans to found chemistry proper, need to make use of theoretical constructs that are already part of the chemistry in the process of being developed. The culturalist approach is thus tainted by a form of circularity of which it claims to be exempt (see Hunger, 2001). Secondly, it is regrettable that, due to this foundation-oriented ambition, Psarros tries to link chemistry to *practices of everyday life*, rather than shedding light on the articulation between the theories of chemists and their *laboratory practices*. Thirdly, in its current state, chemistry is a science that works well: chemists seem to have no trouble communicating and carrying out their research successfully. So why try to modify chemistry by redefining its vocabulary? Fourthly, the anti-realist claim that atoms and molecules are simple theoretical constructions with no counterpart in reality is not justified. It too is an assumption that is just as debatable (for it is just as unverifiable) as the opposing assumption whereby matter is in fact made up on atoms and molecules. Lastly, Psarros's clarification of the role of the atomic model in chemistry remains rather limited.

### 2.3. Outline of a Pragmatic Approach to the Epistemology of Chemistry

I would like to further develop this analysis of the use of the atomic model in chemistry. To do so, let me outline a pragmatic approach that can be effectively applied to chemistry.

Pragmatism, as it was elaborated and developed by Peirce, James, and Dewey, offers an alternative both to scientific realism and to radical versions of anti-realism, insofar as it stays away from some of their claims, which are speculative and unverifiable. This philosophy is a method above all. As Peirce (1998 [1906], p. 400) remarked:

Pragmatism is, in itself, no doctrine of metaphysics, no attempt to determine any truth of things. It is merely a method of ascertaining the meanings of hard words and of abstract concepts.

It is not a question of redefining terms (as Psarros proposed), but of stating what those terms mean in practice, as they are actually used. In other words, what concrete effects are associated with the objects that these terms represent. According to this method, it is not useful to make a statement about whether atoms really do or do not exist. The two ontological assumptions opposed on this point make no difference on the practical level: we have no means of establishing, in a definitive way, that atoms actually have a counterpart in some independent reality.

The principle of the pragmatic approach applied to the epistemology of chemistry can be stated as follows: *leave chemistry alone and explain the connections between the theoretical tools and the practices of chemists, in view of understanding what makes this discipline work.* To this end, I propose a two-step approach (a variation of the pragmatic interpretation of quantum mechanics found in Bächtold, 2008 and 2009):

1. Clarify the goals of chemists in their work.
2. Shed light on the way in which each theoretical (conceptual or mathematical) construct of chemistry enables attainment of those goals, or more specifically (2a) identify the functions that each theoretical construct performs in attaining those goals and (2b) understand how it performs those functions.

According to this approach, the reason for introducing a given entity or mathematical structure into the theoretical framework of chemistry is not some assumed correspondence with an independent reality, but the fact that this entity or this mathematical structure fulfills one or more functions needed for chemists to successfully do their work.

Below, I will present some possible ways of implementing this approach, while looking more specifically at the atomic model on the second step.

## 2.4. Pragmatic View of Chemists' Goals

What goals do chemists attempt to reach in their work? In the literature, we find three types of definitions of these goals:

- (a) The goal of chemistry is to describe and predict the properties of chemical substances and the way in which they react with each other (e.g., see McQuarrie & Rock, 2011, p. 1).
- (b) The goal of chemistry is to describe and predict the properties of atoms and molecules and the way in which they react with each other (e.g., see Lawrence, Rodger & Compton, 1996, p. 1).
- (c) The goal of chemistry is to synthesize new chemical substances (regarding this goal, less often stated, see Schummer, 2006, pp. 32-33; Sjöström, 2007, pp. 85-86).

Let us examine these three definitions. Definitions (a) and (b) refer back to two descriptions of matter—both of which are acknowledged today by chemists—situated respectively on the macroscopic and microscopic levels. At first glance, they appear to be equivalent.

However, definition (b) is faced with two objections. Firstly, it is based on the assumption that the purpose of chemistry is to study entities (namely atoms and molecules) that were not included in the theoretical framework of chemistry until the 19th century and have no guarantee of being maintained in the future. Clearly, because of the underdetermination of the theory by experiment (see above, section 2.1), nothing rules out the possibility that the theory describing the microscopic level (currently quantum chemistry) will itself be replaced in the future by another theory proposing a different description of this level, i.e., one stated in terms of entities other than molecules, atoms, and their constituents, electrons and nuclei. This possibility leads van Brakel (1997, p. 253) to support that “chemistry is not primarily the science of molecules, but of substances.” This objection does not require rejection of definition (b), but reduces its applicability in the history of chemistry: it does not apply to chemistry before the 19th century and it may not apply in the future.

Secondly, as we have seen above (in Section 1.3), reducing the macroscopic description of the properties of chemical substances to the microscopic description of quantum theory in terms of molecules, atoms, and their constituents, is not totally feasible. In particular, quantum chemistry cannot currently predict what new chemical substances will form during chemical reactions. In terms of definition (b) of the goal of chemistry, then, what is the status of such reactions? Isn't one of the aims of today's chemists to be able to predict them? In the end, the goal in definition (b) seems to be subordinate to the goal in definition (a), in such a way that definition (b) can be restated as follows: the goal of chemistry is to describe and predict the properties of atoms and molecules and how they react with each other, in order to be able to describe and predict the properties of chemical substances and how they react with each other. From this angle, the atomic model of quantum chemistry serves as a theoretical instrument that can evolve or be replaced in the future (see first objection above). The idea here is not to say that the atomic model does not really describe matter, but to acknowledge a minimal interpretation of it, that is, an operational interpretation.

Limiting ourselves to definition (a) amounts to ignoring the task of a great number of chemists, which consists of synthesizing new chemical substances. With respect to this task, it seems artificial to make the distinction between the analysis and synthesis of chemical substances. The traditional epistemological view that clearly separates “science” from “applied science” turns out to be somewhat irrelevant when it comes to chemistry. As Schummer (2006, pp. 32-33) puts it:

While philosophers of science have been telling us that scientists aim at a true theoretical description of the natural world, the great majority of chemists [...] have actually been engaged in synthesizing new substances, i.e., changing the natural world. [...] the theoretical concepts of chemistry [...], unlike quantum mechanical concepts, not only predict natural phenomena but also serve as guidance for the production of new substances a million times per year.

For some chemists, then, the goal stated in definition (a) can in turn be regarded as subordinate to the goal stated in definition (c).

Definitions (a) and (c) bring to bear three notions that we will look at from the pragmatic standpoint: “chemical substance”, “property”, and “reaction”. The idea here is to specify their *pragmatic meaning*. I understand the “pragmatic meaning” of a term as “the set of practical effects that can be deduced from it, by all the members of a community, when this [term] is used in a certain context” (Bächtold, 2008, p. 845). In chemistry, the “practical effects” essentially refer to what the scientists can observe as a consequence of their manipulations in the laboratories. Unlike Psarros, our approach will not be normative, but fully descriptive. The pragmatic meaning of a term is not imposed by the pragmatic approach; it is the meaning tacitly shared by all chemists and related to the practical uses of the term.

The various definitions of the term “chemical substance” (or “pure substance”) proposed in the literature all refer to a material body, seen at the macroscopic level, to which is associated one, two, or three of the following characteristics:

- (i) It has specific properties that are observable at the macroscopic level.
- (ii) It has a specific atomic composition (“chemical composition”) and a specific atomic structure (or configuration).
- (iii) It cannot be separated into two (or more) compounds that have different properties and/or different atomic compositions and structures.

Characteristic (ii) seems to stem from the same confusion as the one mentioned above in the discussion of definition (b)’s goal of chemistry. Indeed, determining the atomic composition and structure of chemical substances is regarded as a theoretical means of describing, predicting, and/or synthesizing their properties.

Between the other two characteristics, (i) and (iii), the second appears decisive in defining a chemical substance. Indeed, as emphasized by Schummer (1998, p. 136), empirical knowledge of the properties of a

material body (e.g., melting point, index of refraction, viscosity, acidity, oxidizing power, electrophilicity index...) doesn't enable to say if it is a chemical substance or not. The only means to do so, according to Schummer (*Ibid*, pp. 138-139), is to carry out techniques of material body purification, that is, techniques that separate their chemical compounds. Characteristic (iii) refers to this "operational criterion" (*Ibid*, p. 139). It is by means of "experimental interventions" on the material body under study (causing transition phases) that chemists manage to get a "pure substance" (synonymous with "chemical substance"), which cannot be separated into two (or more) compounds that have different properties and/or different atomic compositions and structures.

We can reverse Schummer's view, and in doing so, partially state the pragmatic meaning of the expression "chemical substance". Knowing that something is a chemical substance means knowing certain observable effects of certain ways of acting upon it. For example, the technique of purifying a chemical substance (i.e., causing a phase transition) does not separate it into chemical compounds with different properties, in such a way that it keeps the same observable properties.

So far, we have only "partially" specified the pragmatic meaning of the expression "chemical substance". And we still need to state the meaning of the term "property" (of a chemical substance). Chemistry textbooks generally do not provide a definition. To help us get an idea on this, let us look at a few examples of properties: colour, density, acidity, oxidizing power, electronegativity, melting point, electrical conductivity, heat of combustion, solubility, index of refraction, electrophilicity index ...

It is for this notion of "property" that the pragmatic approach seems to be the most original, or at least one that does not align with the conception commonly found in chemistry textbooks. According to the latter conception, which can be qualified as "ontological", a "property" of a chemical substance is an attribute of it when it is taken in isolation, i.e., an attribute the substance has no matter what environment it is in and that can be discovered by chemists in their experimental studies.

The pragmatic approach sets aside this ontological view and looks instead at the operational dimension of the properties of chemical substances. As pointed out by James (1995 [1907], p. 71), by virtue of the properties we ascribe to a substance, the latter has a "steering function". For, knowing these properties helps us to "anticipate" the possible observable "consequences" issued from the operations made on the substance under study (1997 [1909], p. 246). For this reason, Dewey (1938, p. 129) writes: "being a substantial object defines a specific function." According to him, the properties of a substance are viewed as

“*potentialities* for specified existential consequences” (*idem*). He gives the following example (*idem*):

The object, *sugar*, may disappear in solution. It is then further qualified; it is a soluble object. In a chemical interaction its constitution may be so changed that it is no longer sugar. Capacity for undergoing this change is henceforth an additional qualification or property of anything that is sugar.

Moreover, when referring to a chemical substance using everyday language (e.g., “carbon dioxide”) or a chemical formula (e.g.,  $\text{CO}_2$ ), chemists are implicitly referring to a set of properties. A chemical substance thus also has an *economy of thought function* (pointed out by James and Dewey following Mach’s influence): it concisely embodies the knowledge chemists have of the observable effects likely to occur when they act upon the substance. As Dewey (*idem*) puts it:

A chemical substance is represented not by enumeration of qualities as such, but by a formula which provides a synoptic indication of the various types of consequences that will result.

Note that when a chemical substance is in the solid state, its chemical formula is sometimes insufficient to encompass all of its properties. The structure of the solid it forms has to be specified. An example of this is solid carbon that, depending on its structure, can come in the form of graphite, diamonds, fullerenes, nanotubes, or graphene. I might add that referring to a given chemical substance does not amount to referring to a particular object, but to a *set* of objects which, when acted upon in various possible ways, all produce the same observable effects. The economy of thought function of a chemical substance is thus twofold.

We are now in a position to list the various aspects of the pragmatic meaning of the term “chemical substance”:

When we refer to a chemical substance we are referring to a set of material bodies:

- that are characterized by the same set of potential observable effects resulting from the various possible ways of acting upon those bodies;
- that cannot be separated into two (or more) material bodies characterized by a different set of potential observable effects resulting from the various possible ways of acting upon those bodies.



What types of actions or manipulations are we talking about when we attempt to identify a chemical substance? On this point, some chemistry textbooks make the distinction between two types of properties of chemical substances: “physical properties” and “chemical properties”. For instance, according to Masterton and Hurley (2009, p. 13):

Substances may be identified on the basis of their:

- chemical properties, observed when the substance takes part in a chemical reaction, a change that converts it to a new substance. [...]
- physical properties, observed without changing the chemical identity of a substance.

For example, according to these definitions, the oxidizing power or the combustion heat of a chemical substance are chemical properties, whereas its melting point and index of refraction are physical properties.

What does this distinction translate into at the pragmatic level? A “chemical property” of a chemical substance is an observable effect of the manipulation of the substance that is *accompanied by changes* in other potential observable effects resulting in other possible manipulations of that substance. In this case, we say that the manipulation causes the chemical substance to take part in a “chemical reaction” (e.g., oxidation or combustion) with other chemical substances (or within that same substance).

A “physical property” of a chemical substance is an observable effect of the manipulation of the substance *that is not accompanied by changes* in other potential observable effects resulting from other possible manipulations of that substance. In this case, we say that the manipulation puts the chemical substance in certain “physical conditions” (e.g., for the fusion point, the temperature or pressure conditions) and/or makes it take part in a “physical interaction” with another physical system (e.g., for the refraction index, interaction with incident electromagnetic radiation; in NMR spectroscopy, interaction with a magnetic field).

This distinction highlights what lies at the core of established knowledge in chemistry: chemical reactions and their associated transformations. From a pragmatic perspective, a “chemical reaction” is the transformation of material bodies into *new* material bodies each having a *new* set of potential observable effects resulting from the various ways in which they can be manipulated. It is the empirical study of these reaction-triggered transformations that allows us to establish the properties of chemical substances.

From this standpoint, relations between chemical substances appear essential in constituting the content of chemical knowledge. As Schummer (1998, pp. 134-135) stressed, the relations studied in chemistry are

relations between substances reacting with each other, but they are also relations between those substances and the products of the reaction. These relations are “dynamic” and “asymmetrical”, which is why some authors attribute epistemological primacy to relations and rank chemical substances as mere theoretical tools for understanding these relations. For example, Schummer (1998, pp. 135 and 140-141) states:

Chemistry at the core is a science of peculiar relations. Instead of isolated objects to be measured, compared and put into a classificatory scheme, dynamic relations between objects constitute the basic set of chemical knowledge, and, at the same time, provide grounds for the classifications of the objects themselves [...] *We need distinct substances as definite starting and end points of chemical reactions, as relata of the chemical relations.* And we need them even more for connecting the relations together in order to build up the chemical network, the logical structure of chemical knowledge.

However, the epistemological primacy granted to relations is just as open to criticism as the epistemological primacy granted to chemical substances. First of all, from a logical point of view, how can we conceive of and study relations without presupposing the existence of *relata*, i.e., objects to be related to each other? Secondly, in practice, chemists use their knowledge of chemical substances and their properties, to establish new relations with other substances, and in doing so enhance their knowledge of the first substances. Hence, knowledge about relations serves to construct knowledge about chemical substances, just as much as the latter allow us to construct the former: this knowledge is built jointly (i.e., chemical substances and their relations with each other are determined in a co-dependent way).

In addition to the importance of relations in building chemistry knowledge, the attention of pragmatic epistemologists interested in chemistry is attracted to the changes taking place during the chemical reactions associated with those relations. In chemistry, as in physics, knowledge is not built from the simple observation of the objects under study, taken in isolation, but by acting upon those objects and observing the resulting effects, i.e., by interacting with them. The thing that makes chemistry differ from physics seems to lie in the *changes* generated by chemists' actions: knowledge building rests on these transforming actions. This specificity explains why, in the field of chemistry, the boundary between “science” and “applied science” is fuzzy. The transforming actions of chemists have an epistemic facet and a technological (or technoscientific) facet. They permit the acquisition of knowledge, and thus the pursuit of the goal stated in definition (a), as much as they enable the

production of new chemical substances with various different uses and hence the pursuit of the goal stated in definition (b).

## 2.5. Pragmatic Look at the Roles of Classification and the Atomic Model

The second step of the pragmatic approach outlined above has two sub-steps: (2a) identify the functions that each theoretical (conceptual or mathematical) construct performs in reaching the goals of chemistry, and (2b) understand how it performs those functions. It is beyond the scope of this paper to conduct an investigation for each theoretical construct of chemistry. I will simply suggest a few avenues for one particular construct, namely, the atomic model.

In order to situate the functions of the atomic model, we must first determine the functions of the chemical classification the model enables to reconsider. Classifying chemical substances and defining a corresponding nomenclature is one of the main theoretical tasks of chemists (e.g., see Schütt, 2003). Chemical substances are currently classified as simple substances (e.g., carbon, oxygen, etc.) and composite substances or “compounds”, themselves grouped into “families” (e.g., acids, alcohols, etc.), subfamilies, and so forth (classification of the IUPAC<sup>5</sup>). What is the utility of this classification? At least four functions can be identified:

- (A1) *A unifying function.* The classification groups together into families, subfamilies, etc., a large number of chemical substances that have similar chemical properties. The pragmatic approach translates these properties into similar potential observable effects resulting from some of their possible manipulations.
- (A2) *An economy of thought function.* This function is correlated with the unifying function, since classifying chemical substances into families, subfamilies, etc., provides a concise way of referring to a very large number of chemical substances with similar chemical properties (the classification thus increases the economy of thought already afforded by the chemical substances).
- (A3) *A communication function.* By virtue of the unifying and economy of thought functions it fulfills, the classification allows chemists to make sure they are referring to the same substance, which is not self-evident given the high number of known chemical

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<sup>5</sup> IUPAC, International Union of Pure and Applied Chemistry, see <<http://www.iupac.org/>>.

substances (in January of 2012, the CAS<sup>6</sup> listed 64 million). This function allows chemistry research to be carried out collectively.

- (A4) *A description and prediction function.* The classification is able to perform this function because it performs the unifying function. Knowing that a chemical substance belongs to a given family allows one to describe and predict the potential observable effects resulting from some of its possible manipulations, namely, those that characterize the chemical substances of the family in question. By that token, the classification enables one to pursue the goal of chemistry stated in definition (a). In addition, gaps in the classification allow one to predict the existence of unknown chemical substances (see Schummer, 1998, p. 144)

Note that to establish the classification systems and nomenclatures that have succeeded each other in the recent history of chemistry (in the 20th century), pragmatic requirements (pertaining to the fulfillment of specific functions useful for chemists) set the pace in terms of systematicity (see Bensaude-Vincent 2003, p. 188).

To attain the goals of chemistry stated in definitions (a) and (b), isn't it sufficient to propose a relevant classification? Couldn't chemists do without atom-based representations of chemical substances? Apparently not, firstly, because the atomic model provides the guidelines for doing the classification, and secondly, because it considerably increases the classification's descriptive and predictive power. More specifically, the atomic model fulfills the following functions:

- (B1) *A data-relating function.* The atomic model allows one to define a network of relations between large sets of empirical data about chemical substances (or observable effects resulting from chemists' manipulations) compiled in chemistry. On this point, Cassirer (2003 [1910], p. 209) uses the expression "circle of empirical relations" and goes on to say that the concept of atom (and of molecule, with its different possible spatial representations, I should add) acts as a "mediator" with respect to empirical data.
- (B2) *A unifying function.* Once interrelated in terms of atoms and molecules, massive amounts of diverse empirical data can be translated and incorporated into one and the same theoretical structure.
- (B3) *An economy of thought function.* This function is correlated with the unifying function, since assembling empirical data by relating

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<sup>6</sup> Chemical Abstracts Service, see <<http://www.cas.org/>>.

them to atoms and molecules allows one to refer to these data in a concise manner. The atomic model thus enhances the economy of thought already afforded by the chemical substances.

In line with Cassirer, Llored talks about these two correlated functions, unification and economy of thought, based on his study of Mulliken's contribution to the development of quantum chemistry. For Llored (2010, p. 218), the concept of atom is a tool that condenses and unifies multiple relations between empirical data, as illustrated by Mulliken's correlation diagrams, which are said to provide a good example of this unifying ability. It would seem, then, that it is because the atomic model satisfies these two functions that it acts as a guide for classifying chemical substances.

(B4) *A description and prediction function.* Because it interrelates and unifies empirical data about chemical substances, the atomic model offers a theoretical framework for describing these data and predicting the result of future experiments involving chemical substances. In doing so, the atomic model allows one to pursue the goal of chemistry stated in definition (a).

As we see, the different functions of the atomic model are interconnected. The question that remains is: How does this model fulfill these functions? Here are some possible answers.

- *The nuclei of atoms (as well as their core electrons) offer a pole of stability.* The chemical reactions studied in chemistry involve transformations of the chemical properties of the concerned material bodies (or in pragmatic terms, changes in the potential observable effects resulting from possible manipulations of those bodies). The nuclei (and their core electrons) used to describe these bodies offer a pole of stability with respect to these transformations. They thus allow us to grasp the links between the chemical properties of the reactants and those of the products of the reactions.
- *The atomic model is universal.* According to the atomic model, all chemical substances are made up of atoms belonging to a limited set of different types of atoms (approximately 100), all of which have the same kinds of constituents (electrons and nucleons). This universality supplies a theoretical framework for understanding the links between chemical substances whose chemical properties are similar and who belong to the same family. If, as Cassirer

contended (2003 [1910], p. 208), “the atom functions here as the conceived unitary center of a system of coordinates, in which we conceive all assertions concerning the various groups of chemical properties arranged”, then it is by virtue of its invariance and universality.

- *The atomic model is easy to manipulate mentally.* Whether they take on the form of letters, for example, or of mental images of little balls, the symbols used to stand for atoms and their constituents (electrons, protons, and neutrons) are objects that are easy to use in performing many mental operations. It is thus possible to think of making and unmaking various combinations, with bonds of various types (repulsive or attractive, weak or strong, etc.). Borrowing Malrieu’s (2008, p. 8) image, the atomic model in chemistry is analogous to a “molecular game of Lego”, being both very simple and potentially very powerful. It should be noted that if this model is so easy to manipulate mentally, it is notably because atoms and thus molecules can be represented figuratively by simple diagrams (two- or three-dimensional). There are various ways of diagramming molecules (see for example the different diagrams of camphor in Hoffmann & Laszlo, 1991, pp. 4-5, or butadiene in Nye, 1993, p. 280); each is useful for treating a particular aspect of the properties and reactions of chemicals, each is “suitable for some purposes” (Hoffmann et Laszlo, 1991, p. 5), or as stated by Bensaude-Vincent & Simon (2008, p. 206): “Whether planar or three dimensional, the primary purpose of such chemical formulae is not to represent the structure of molecules, but to predict behaviour and to help in the construction of new molecules.”
- *The atomic model can be expanded in multiple ways.* It is highly flexible, i.e., it can readily be extended or modified to include new hypotheses (e.g., role of electrons in chemical bonds) and/or a mathematical structure (e.g., a wave function of quantum mechanics describing a molecule’s electrons), whether for the purposes of integrating new empirical knowledge or adapting to it. In fact, the atomic model used during the 19th and 20th centuries to describe and predict chemical properties and reactions evolved considerably during that period, going from Dalton’s simple, minimal model to the complex, rich model of quantum chemistry, after passing through Lewis’s model. Moreover in present-day chemistry, the exact hypotheses that constitute the atomic model employed today can be adapted to fit

the experimental conditions (e.g., collisions of the modeled molecule with other molecules, presence of an electromagnetic or gravitational field, etc.) or as Zeidler (2000) puts it: “The application of a specific model of molecular structure depends on the kind of experiments that we want to describe by the use of a model.”

## Conclusion

According to the argument of the underdetermination of the theory by experiment, the ontological question as to whether matter is *really* composed of atoms cannot be answered. What we can know about material reality at the microscopic level is based solely on observations of the effects of our actions on that reality. This being the case, the atomic model stands out as the best theoretical tool currently available for describing and predicting these observations. This is especially true in chemistry, where one of the goals is to describe and predict observable effects resulting from actions that transform the objects under study. In this respect, the pragmatic approach strives to offer a framework for thinking about and understanding why chemists use the atomic model: instead of trying to establish a presumed correspondence between the model and an independent reality, what we want to do is shed light on the functions that it fulfills in reaching this goal of chemistry.

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# THE TAO OF CHEMISTRY

ANDREW PICKERING

A conception is needed which overcomes the one-sidedness that necessarily arises when limited intellectual processes are detached from their matrix in the total activity of society.

—Max Horkheimer (1972, 199).

Chemistry was my first love in science. I loved the brilliant colours of pure chemicals, the jewel-like crystals growing in beakers, the magical changes of state: the ‘flocculent white precipitate’ that appears like a snowstorm from nowhere when an intensely blue solution of copper sulphate mixes with colourless sodium hydroxide; the slow dissolution of my school uniform under a rain of acid splashes. Our chemistry lab was the Shangri-la of Coventry. None of this registers very well in academic history, philosophy and sociology of chemistry. Chemistry studies, to coin a phrase, remain largely under the spell of studies of physics (my second love), obsessed with knowledge, theory and the problematics of epistemology.<sup>1</sup>

In contrast, this essay explores possibilities for an ontological turn, by developing ways of thinking and writing that can bring the materiality of chemistry and chemicals into focus.<sup>2</sup> I use ‘ontology’ here in a very general sense, as concerning how things are in the world and how they go. Much of what I have to say is obvious, but the obvious tends to escape from academic view. I think of a gestalt switch in which the ‘obvious’

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<sup>1</sup> My schoolboy relationship with chemistry came to an end when we moved on to organic chemistry. I hated the peculiar smells and took to hanging out with physics instead. Put off by high-voltage shocks, my life took an epistemological turn and I increasingly spent my time with equations. Later I fled the thin pleasures of disembodied attachment into the arms of science studies.

<sup>2</sup> For work that goes in similar directions to this essay but with much great historical specificity, see the work of Ursula Klein et al, for instance Klein (2005, 2010, this volume), Klein and Lefèvre (2007), Klein and Spary (2010). See also Baird (1993, 2004) on the role of chemical instrumentation.

background to chemistry moves to the foreground of attention and invites a reconsideration of traditional epistemological topics.

Running through the essay is a concern with the specificity of chemistry. Theoretically, the overall perspective derives from my own work on ‘the mangle of practice,’ based on the analysis of research practice in physics (Pickering 1995), and ‘posthumanist’ science studies more generally (Pickering 2008a). Empirically, my claim to scholarly knowledge of this area derives from my work on the development of organic chemistry and the synthetic dye industry in the later 19th century (Pickering 2005). My examples are often drawn from that study, though I think the discussion has wider relevance.

### **Sensuous Matter**

If physics concerns itself with a homogeneous though invisible world, then chemistry is immediately about a world that is visibly differentiated and heterogeneous, containing all sorts of different kinds of stuff: solids, liquids, gases, 92 stable elements, metals, salts, polymers . . . And if physics dwells endlessly on the primary qualities of space, time and matter, chemistry pertains directly to the mundane world of secondary qualities like colours and tastes. Dyes, for example, are all about making cloth look pretty. Chemicals also engage with our bodies in a way that the objects of physics do not. Food nourishes us; some foods aid digestion; other substances interfere with mental processes and diseases. We have, that is, a continuous bodily engagement with the heterogeneous entities that make up the ontological field of chemistry. It seems right to argue that these bodily engagements have been and continue to be the surface of emergence for distinctly chemical endeavours down the ages.<sup>3</sup>

### **Material Agency**

If epistemology is about knowledge and representation, the ontological turn is marked by a concern with agency and performance, and in this respect chemistry is an obvious reference point for science studies. If the

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<sup>3</sup> I take the phrase ‘surface of emergence’ from Michel Foucault’s (1972) discussion of the emergence of specific discourses from non-discursive substrates (such as the prison) (Pickering 2005). In Foucault’s sense, Klein discusses the emergence of chemistry from pharmacy and dyeing; Spary studies chemistry’s relation to high-class food and drink; drawing on the work of others, my own work continues the story of chemistry and the dye industry into the later 19th century (opera cit, note 2).

forces of physics are the invisible springs of worldly events, chemicals are visibly active in their own right. I mentioned the disintegrating effects of acids on my clothing as a schoolboy. At the heart of the Industrial Revolution in the West was the textile industry, and at the heart of that was the bleach that turned wool white, and the mordant chemicals that bit into it and rendered it susceptible to the dyes that coloured it again. The powers and agency of material substances are what chemistry is about. And we should note that our human concern is not with agency in the abstract, but again with agency as it bears on us—with chemical actions like bleaching and dyeing that matter to us phenomenologically and economically.

We should think more about heterogeneity here. Matter acts on matter, but not on itself. Sulphuric acid did interesting things to my school uniform, but nothing much happens if you mix the contents of two beakers of sulphuric acid together. Much chemical practice thus consists in maintaining and even intensifying material heterogeneity, often with the intention of uniting different substances at an appropriate time and place to achieve a desired end. A devotion to chemical purity is the obverse of material agency as a surface of emergence for chemistry. We could think of chemistry as an intricate orchestration or choreography of material identities, differences and performances.<sup>4</sup>

## Transits of Matter

Chemistry has never been satisfied with the world as found. From ancient traditions of alchemy around the world to the hi-tech industry of today, chemists have sought to transmute matter, creating new substances and increasing the heterogeneity of the world—by exploring the agency of existing substances in acting on one another, or through processes of solution and distillation, or the use of fire. These transits of matter are at the heart of chemistry, and we need to think further about them.

A key point to note is that the chemists do not control these transits or the agency of their products; they cannot will them into existence.

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<sup>4</sup> There is a sort of material parallel here to the second law of thermodynamics—specific chemical effects can only be obtained from specific chemical differences—though oddly it is hard to think of any discussions of a chemical equivalent to the 'heat death' of the universe. See also Latour and Woolgar's (1986) insightful discussion of the importance of labels on samples in a biology laboratory. If one removed the labels, research would come to a halt. Charis Thompson (2005) speaks of 'ontological choreography,' though her concern is with the different subject positions taken up by humans in different contexts.

Chemistry is about finding out what matter will do. A key event in the history of organic chemistry was the discovery of one of the first synthetic dyes, mauve, by William Henry Perkin in 1856. Perkin's explicit goal was to find an artificial way of producing the anti-malarial drug quinine. It just so happened that combining certain chemicals in certain ways he arrived at a substance capable of transmitting a brilliant colour to cloth. One way to register this fact is to point to the emergent quality of such transits: no one can know where they will lead except by trying them out. Chemical research thus has the quality of an open-ended performative search in the space of material agency.

And we, too, are bound up and transformed in this search. It takes the form, as I would say, of a dance of agency, a decentred back and forth between the human and the nonhuman, in which each partner alternates between activity and passivity and is constitutively reformed in the process (Pickering 1995). Just as a new kind of stuff, mauve, emerged in Perkins' experimentation, so did a new sort of business opportunity, transforming Perkin from a young student of chemistry to a major figure in the new synthetic dye industry. More generally, our social and economic landscape has been increasingly configured around the emergent footholds on nature that have appeared in work like Perkins'. Think of the extent to which the world today depends on just a few of these: plastics, explosives, fertilisers, synthetic dyes and their latter-day descendants, pharmaceutical drugs, for example. If the mundane material world is a surface of emergence for chemistry, then it is also a surface of return.

## **The Laboratory**

To speak of the mundane world as a surface of emergence and return is to conjure up a vision of chemistry as to some extent separate from the everyday. For centuries, the laboratory has been the material locus of this separation, a place where heterogeneous materials can be subjected to trials and transformations never before encountered in nature or routine human activity (Latour 1987). So we should think of another sort of transit of matter, now into and out of the laboratory. And we should recall that successful transits out of the lab are just as chancy and emergent as the new transits established within the lab. To exploit the commercial potential of his discovery, Perkin had to scale up the mauve synthesis to produce industrial quantities of the dye, and this, too, opened up new dances of agency which proved hazardous in the extreme. Chemists were killed and injured in explosions and fires that broke out when the process was scaled up. Again, it just so happened that Perkin and others found

ways to keep the synthesis under control at an industrial scale. They might have failed; the synthetic dye industry might not have existed.

## Flows

We need to think about space. Chemistry is situated in a complex pattern of material flows from one place to another. At the microlevel, for example, materials flow into and out of the laboratory. In 19th-century organic chemistry, many pure chemicals for academic experimentation were provided by the synthetic dye industry. At the other extreme, chemistry intervenes in macroflows of matter. Before the mid-19th century, most dyes were extracted from vegetables. The macroflow went from fields through extraction plants to cloth to the consumer. The coming of synthetic dyes strangled that flow and established another one, now linking coal mines via the production of coal tar and chemical factories, with a detour through the lab, to dyers and the consumer. These macroflows are, needless to say, of great social and economic significance. The synthesis of artificial equivalents put madder farmers and indigo planters out of business, and established the German and Swiss dye companies as a major feature of the industrial landscape, now even more powerful as ‘big pharma.’

Here, too, we can understand chemistry as engaged in a sort of material choreography, intervening in macroflows of matter punctuated by transmutations of form along the way. And we should remember that these megafloWS are again never fully subject to human control. There is always some degree of leakage and of the production of unexpected and emergent new flows. Arsenic was a key ingredient of the manufacture of early synthetic dyes and refused to be confined to dye-works—appearing instead in ground water around the plants, poisoning and killing workers in their homes. Freons make refrigerators work, but also flee to the upper atmosphere and make holes in the ozone layer. Organic chemicals like oil make transits into carbon dioxide when burned, upsetting the thermal balance of the planet. Pollution is the emergent other side of the chemical orchestration of nature.<sup>5</sup>

## Knowledge

I have been trying to thematise the materiality of chemistry, but we can turn to its epistemic dimension, the traditional focus of chemistry studies.

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<sup>5</sup> See Caillol, Godard, and Rico-Lattes and Laura Maxim, this volume.

How should we think about the chemical knowledge of formulae, analyses and syntheses that have been the trademark of academic chemistry for at least the past 150 years? The answer, I take it, is that chemical knowledge is itself bound up with flows and transits of matter. In the history of organic chemistry, no obvious intrinsic rightness attached to the overall form of Kekulé's benzene-ring theory, or to particular molecular assignments within that frame. What one can say is that Kekulé's theory fitted in better in specifiable ways with chemists' explorations of the sorts of transits of matter relevant to the dye industry. And at the microlevel, the rightness or wrongness ascribed to molecular formulae was a function of how well they made sense of earlier syntheses and fed into new ones. Scientific knowledge, then, itself grew and evolved in a mangle-ish fashion in a constitutive interrelation with the growth and evolution of the space of transits and flows of matter (Pickering 2005).

Chemical knowledge, one can say, grows as part of a heterogeneous material, social and conceptual assemblage—increasingly an integral part of that assemblage, but never its controlling or generative centre as traditional history and philosophy of chemical ideas implicitly suggests. And the philosophical and historiographic moral of this is that we can never get a secure grip on what chemical knowledge is without at the same time taking account of the specific flows and transits and the wider socio-economic assemblage with which it engages—which takes us back to the epigraph from Max Horkheimer.

## The Tao

I have sketched out an image of chemistry as an orchestration of flows and transits of matter that we cannot control but that we can learn to incorporate in human life and build our lives around. If one wanted to trace out a philosophical genealogy for this image, where might one look? Certainly not to analytic philosophy of science with its disembodied focus on ideas and representations. Perhaps to the philosophy of Gilles Deleuze and Felix Guattari (1987) as developed further in the writings of Manuel DeLanda (2002, 2005), with its emphasis on the emergent agency of things and its ontology of heterogeneous assemblages. Perhaps to the historical materialism of Marx (and Horkheimer again), and the early Marxist fascination with, indeed, the synthetic dye industry. But all of this work echoes back towards earlier and premodern ontologies, and the



philosophical schema that best catches up the overall picture developed in this essay is, I think, Taoism.<sup>6</sup>

The ontology of Taoism is, in many ways, the same as that ascribed here to chemistry. The basic Taoist image is that of a heterogeneous world always in flux, a place of emergent flows and transformations. Taoism likewise insists that humanity is just a part of this world, doing its best to get along with the flows and certainly not in control of them. And *tao*, of course, means path. Taoism is an ontology of paths, and the argument here is that chemistry is all about making, finding and following paths—precisely the transits and flows that have been under discussion.<sup>7</sup>

Taoism, then, offers us an excellent ontological framework for thinking about chemistry. And yet this suggestion seems incongruous, and it might be instructive to analyse why that is. Various lines of thought present themselves. At the level of articulated knowledge, the self-understanding of chemistry (and all the modern sciences) denies any

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<sup>6</sup> The title of my essay obviously derives from Fritjof Capra's classic work, *The Tao of Physics* (1976), but it is worth noting that we make connections to the East in different ways. Capra makes the link by comparing philosophical statements from quantum physicists and Eastern philosophers, often, though not always, statements concerning epistemology and the limits on our ability to know the world. My strategy is instead to point to the material world and the place of chemistry in it. Capra, in fact, draws on many Eastern traditions, while I refer here to Taoism in particular. My knowledge of Taoism is limited and what follows adopts a minimalist interpretation of Taoist ontology, but it seems to me that Taoism is especially relevant amongst Eastern traditions as a posthumanist philosophy that is not centred on notions of transcendence and escape from the shackles of the material world (in contrast to Buddhism). Jullien's (1999) discussion of the Chinese concept of *shi* as a potential for action is very relevant here; see also Scheid (2002) on contemporary versions of traditional Chinese medicine. For more on East-West ontological connections, see Pickering (2011). For another paper called 'The Tao of Chemistry,' see Scerri (1986). Like Capra, Scerri is concerned by parallels between taoist ideas and concepts from chemical theory; I thank him for sending me a copy of his paper.

<sup>7</sup> Adrian Cussins (1992) is one of the few Western philosophers to have focussed on paths and 'trails,' as he calls them, in science, though his arguments again circle around epistemic concerns. An interesting question that comes up here concerns the Taoist idea that one should 'go with the flow' and act in conformity with what Jullien (1999) calls the 'propensity of things.' How does one know where the flow is going? I think that in classical Taoist thought such knowledge is the product of experience. In chemistry (and modern science in general) we can be more precise: performative experimentation with chemical substances maps propensities. Perhaps then I should speak of a neo-Taoist understanding to acknowledge this point.

affiliation to the Tao. Chemistry offers us a vision of a world characterised not by endless emergent flows and transmutations, but of fixed invisible entities—atoms and molecules—having fixed properties that we can know and control. At the level of practice, chemistry aims to fix the paths, to regularise the choreography of flows and transits and put them reliably at our disposal—to put humanity at the centre. And this mastery is evident in our daily world: the chemical plants and products are just there, churning out the plastics, explosives and drugs that modernity lives on, and echoing back to us the non-Taoist ontological self-understanding of the science itself.

How should we think about this? First, we have to recognise that chemistry is in this sense a profoundly non-Taoist science. None of this ancient philosophy informs modern chemical thought. One might almost say that the power of chemistry depends upon not recognising any relation to the Tao. The telos of chemistry is to stifle becoming and to split us off from the material world, to make the world more dual (Pickering 2009). And yet I have just argued that the world of chemistry is a Taoist one, whether the chemists (and the rest of us, including people in chemistry studies) recognise it or not. Chemical flows and transits and the knowledge that accompanies them do emerge and become in a decentred process that we do not control, and one can easily see that empirically in all the surprises, leakages, disasters and unexpected environmental effects that have always dogged the field and the industry. The best one can then say, I think, is that chemistry inhabits, and indeed constitutes, a Taoist world, but in a deliberately non-Taoist fashion.<sup>8</sup> To switch to another nonmodern ontology, chemistry inhabits a Heideggerian world of revealing (as do we all), but in the flow of revealing it adopts a stance of mastery and domination—‘enframing’, as Heidegger (1977) called it, rather than poiesis (Pickering 2008b).<sup>9</sup>

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<sup>8</sup> I am not sure how express this point in Taoist terms. Perhaps one would say that Yin and Yang have got out of balance in modern chemistry, with the masculine ordering principle, Yang, overwhelming its feminine counterpart. Some principle of cosmic balance would then suggest that the pendulum will eventually move in the opposite direction, and perhaps the developments discussed below (and me writing about them) offer some inkling of this process. This gendered imagery is alien to me, but not without empirical referent. See, for example, Wise and Brock's (1998) account of a conference at Princeton University where critics of the sciences of complexity repeatedly invoked images of children, kitchens, zoos and animals (Pickering 2010, 436n70).

<sup>9</sup> I take it this is a concrete exemplification of Latour's (1993) characterisation of modernity in terms of an effective obfuscation of emergent, decentred intertwinings of the human and the nonhuman, but Latour's characterisation of

## Taoist chemistry

All of which is to invite the question of whether one might have a chemistry that acknowledges its Taoist situation rather than denying it. The temptation here is to look backwards. It would no doubt be instructive to compare ancient Chinese chemistry with its modern Western counterpart (Needham 1981), though this task is beyond me at present. One could also think of the many traditions of premodern alchemy that have flourished all around the world, including Taoist alchemy. The Western alchemical tradition, for example, centred on coupled transformations of the alchemist and matter—precisely the sort of posthumanist decentering that modern chemistry denies.

It might also, however, be useful to end this essay by looking at contemporary echoes of Taoism within chemistry proper.<sup>10</sup> I think here of intersections between chemistry and the wider sciences of complexity. Again, I cannot produce a coherent overview, but a few examples might convey the overall line of thought. Nobel laureate Ilya Prigogine comes to mind.<sup>11</sup> If mainstream chemistry is about systems close to equilibrium from which novelty is largely absent, the focus of Prigogine's work is on the surprising properties of matter far from equilibrium. 'Extreme sensitivity to initial conditions'—the 'butterfly effect'—points to the limits of human prediction and control and to the emergent liveliness of nature, and thus returns us to a Taoist perspective on materiality. Systems biology has likewise come to grapple with the non-machinelike emergent properties of immensely complex assemblages of molecules (Moss forthcoming). If those problematic are largely epistemological, at a more material and directly ontological level I think of empirical research focussed on the self-organising properties of matter—Bénard cells, the Belousov-Zhabotinsky reaction—that again confront us with a Taoist liveliness of nature and a generation of form independent of human input.

Finally we could leave the laboratory for the 'artworld'. Figure 1 is a photograph of a dynamic assemblage called 'Electrochemical Glass' by

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Martin Heidegger's philosophy has recently been at the centre of debates in posthumanist science and technology studies: Jensen (2006), Kochan (2010), Pickering (2009), Riis (2008).

<sup>10</sup> From the outside, the uncontrolled flows around chemistry are already apparent: Beck (1992). The standard temptation is to regard this lack of control as the product of culpable human error. From a Taoist (or Heideggerian) perspective, the ability of the world to evade our control is an ontological fact—which is not to deny that human errors and other failings exist.

<sup>11</sup> See Prigogine and Stengers (1984) for an accessible introduction.

the Edinburgh-based artist Richard Brown. Here three electrodes of copper, aluminium and iron were sandwiched in a conducting fluid between two glass plates and evolved over time into a continuously changing work of art.<sup>12</sup> In a conference description, Brown (2003) emphasised the unexpected appearance between April and October 2002 of the black ‘dendrite’ climbing up the left hand side. This work again confronts us with a vision of chemistry as occupying a space of emergent flows and becomings, but now as art rather than science. Brown (2003, 20) discussed this work, ‘as a daily reflection of process, decay, transmutation and growth; the slow changes resonating with memory and notions of self—a form of contemplative alchemy,’ but he might equally have invoked the Tao.

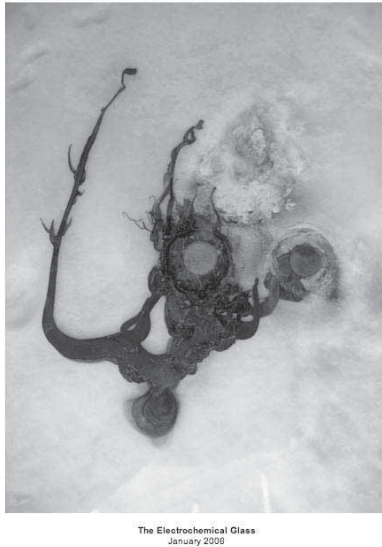


Figure 1: The electrochemical glass, brown (2003)

I began this essay by thinking about a gestalt switch in chemistry studies that would foreground the materiality and becoming of its flows and transits. These neo-Taoist examples from contemporary chemistry

<sup>12</sup> A time series of coloured stills of Electrochemical Glass can be found at [www.mimetics.com/chem/chem1.htm](http://www.mimetics.com/chem/chem1.htm). A single coloured image can be found at the website of the 2008 *Pask Present* exhibition in Vienna: [paskpresent.com/exhibition/?page\\_id=24](http://paskpresent.com/exhibition/?page_id=24); see Glanville and Müller (2008).

point towards a change of gestalt within the field itself, a reversal of figure and ground that promises, not to displace mainstream chemistry, but, in several senses, to put it in its place—to show that it is one way but not the only way for us to live in and know the chemical cosmos. They also take me back to the Shangri-la of Coventry.

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# COMPLEMENTARY CHEMISTRY

HASOK CHANG

What can we possibly gain from taking a philosophical perspective on a well-established scientific discipline such as chemistry? One might imagine that there is legitimate room for external commentary only in the case of those sciences that are still on uncertain ground (such as, say, quantum gravity, the biology of social insects, or the various sciences of well-being) where, perhaps, the professional skills of philosophers can be helpful in untangling messy conceptual knots, or assessing which experiments really provide reliable data, or elucidating the degree and kind of empirical support that contentious theories can claim from available data. In contrast, it would seem that a science like chemistry has no need for a philosophical tune-up: its concepts are cogent, its problems well defined, its facts secure, and its methods well established. In fact chemistry is such an uncontentious science that students may even find it dull and boring.

Of course such a cut-and-dried image of chemistry does not quite fit the realities of chemical practice, and many other chapters in this volume locate and explore various places where interesting philosophical questions concerning chemical concepts and methods do arise. I myself sometimes aspire to do such philosophical work. However, the aim of this paper is to articulate and illustrate a rather different vision of the task of the philosophy (and history) of chemistry. In previous publications I have advanced the notion of “complementary science”, which employs the methods and resources of history and philosophy of science in order to address scientific questions that science itself neglects (e.g., Chang 2004, chapter 6). In the present paper I would like to argue that chemistry is a particularly apt subject for complementary science, and illustrate this claim through a discussion of some striking cases. First I begin with a brief exposition of the general enterprise of complementary science.

Complementary science seeks to generate scientific knowledge in places where science itself fails to do so. This is not to deny that science is very good at what it does, but just to note that there are things that science does not do, even though they are quite scientific. What I refer to here is



not a shortcoming of science; on the contrary, the more well-defined and focused specialist science becomes, the more exclusive and exclusionary it tends to turn. This is a lasting insight from Thomas Kuhn's reflections on the nature of paradigm-based "normal science" (Kuhn 1962). A need for complementary science arises from the fact that specialist science cannot afford to be completely open. (I speak of "specialist science" rather than "normal science", so as not to distract those who reject Kuhn's particular ideas about normal science or paradigms.)

There are two aspects to this necessary lack of openness. First, in specialist science many elements of knowledge must be taken for granted, since they are used as foundations or tools for studying other things. This also means that certain ideas and questions must be suppressed if they are heterodox enough to contradict or destabilize the taken-for-granted items of knowledge. Such are the necessities of specialist science, quite different from a gratuitous suppression of dissent. Second, not all worthwhile questions can be addressed, if only because there are limits to the number of questions that a given community can afford to deal with at a given time. Each specialist scientific community will have some degree of consensus about which problems are most urgent, and which problems can most plausibly be solved. Those problems that are considered either unimportant or unsolvable will be neglected. All this is not malicious or misguided neglect, but a reasonable act of prioritization.

All the same, we must face up to the fact that suppressed and neglected questions do represent a loss of knowledge, actual and potential. The complementary function of history and philosophy of science is to recover and even create such questions and, hopefully, some answers to them as well; what is desired is an enhancement of our knowledge and understanding of nature. Complementary science can address critical questions concerning present science, recover useful ideas and facts from past science, and explore alternative conceptual systems and lines of experimental inquiry for future science. If these investigations are successful, they will complement and enrich current specialist science. Complementary science can enlarge and deepen the pool of our knowledge about nature. In other words, it can *generate* and *improve* scientific knowledge. There are three main ways in which this can be achieved.

*Critical awareness.* Critical philosophical scrutiny can enhance the quality of knowledge. If something is actually uncertain, our knowledge is superior if it embodies an appropriate degree of doubt rather than blind faith. If the reasons we have for a certain belief are inconclusive, being aware of the inconclusiveness prepares us better for the possibility that

other reasons may emerge to overturn our belief. With a critical awareness of uncertainty and inconclusiveness, our knowledge reaches a higher level of flexibility and sophistication. Even philosophers tend not to recognize critical awareness and its productive consequences as contributions to scientific knowledge; thereby philosophy undersells itself. There is a sense in which we do not truly know anything unless we know how we know it, even though certain aims in life require a non-questioning application of knowledge. For example, there is little that deserves the name of knowledge in being able to recite that the earth revolves around the sun. This belief carries more intellectual value if it is accompanied by the understanding of the evidence and the arguments that convinced Copernicus and his followers to reject the firmly established, highly developed and eminently sensible system of geocentric astronomy established by Ptolemy. This is exactly the kind of scientific knowledge that is not easily available in current specialist science but can be given by complementary science, or, history and philosophy of science in its complementary mode. There are many cases in which philosophers and historians have raised and examined very legitimate questions about how certain scientific controversies were settled. In the thriving tradition in the philosophy of modern physics, for instance, a community of philosophers have been questioning and re-examining the orthodox formulations and interpretation of various theories, especially quantum mechanics.

*Recovery.* Once critical awareness about science is reached, history of science takes on an entirely different kind of significance. History can teach us about nature through the recovery of forgotten scientific knowledge. The potential for such recovery is shown, for example, in my recent work on temperature (Chang 2004, chapter 1), which began with a philosophical question about how the so-called "fixed points" of thermometers can be demonstrated to be constant, in the absence of points that are previously agreed to be constant. This question led me to locate a significant debate in history. Many investigators starting with Jean-André De Luc in the late 18th century knew that pure water did not always boil at the "boiling point" even under standard pressure. They built up a growing and sophisticated body of knowledge about the "superheating" of water and other liquids that took place under various circumstances. In some simple experiments I have been able to confirm the most important of these phenomena (Chang 2007). But by the end of the 19th century we witness John Aitken's complaint that authoritative texts were neglecting this body of knowledge, either through ignorance or through oversimplification. Today the relevant specialists do know that liquid water can reach temperatures beyond the normal boiling point without boiling,

and standard textbooks of physical chemistry often mention that fact briefly. Much less commonly noted is the old observation that water that is actually boiling can have various temperatures deviating from the standard boiling point, which seems to be discussed only by engineers concerned about heat transfer. There are vast numbers of scientifically educated people today, including many professional scientists, who do not know anything about these very basic and important phenomena. In fact, what many claim to know is that superheating does *not* happen, when they unsuspectingly recite from their textbooks that pure water always boils at 100°C under standard atmospheric pressure. The recovery of forgotten knowledge is not restricted to facts, but extends to ideas as well (and it is, after all, very difficult to separate facts and ideas cleanly). Come to think of it, historians of science for many decades have made great efforts to recover all sorts of ideas that have been forgotten by modern science. This kind of recovery is the mainstay of the history of science, so much so that there is no point in picking out a few examples out of the great multitude. However, the works of Lawrence Principe and William Newman deserve a special mention (e.g., Newman and Principe 2002), as they have forged a rare and exemplary path of factual and conceptual recovery.

*Extension.* Recovery and critical awareness are valuable in themselves, but they can also stimulate the production of genuinely novel knowledge. Historians have generally shrunk from further *developing* the systems of knowledge that they uncover from the past record of science. An emblematic example is Kuhn. Having made such strenuous and persuasive arguments that certain discarded systems of knowledge (e.g. Aristotelian physics, Ptolemaic astronomy, or the phlogiston theory) were coherent and not simply incorrect, Kuhn gave no explicit indication that these theories deserved to be developed further. Why not? According to his criterion of judgement, scientific revolutions constitute progress when the newer paradigm acquires a greater problem-solving ability than ever achieved by the older paradigm. But how do we know that such superiority is not merely a result of the fact that scientists abandoned the older paradigm and gave up the effort to improve its problem-solving ability? A similar question also arises at the conclusion of some other historians' works on scientific controversy. For example, Steven Shapin and Simon Schaffer, in their *Leviathan and the Air-Pump* (1985), strongly challenged the received wisdom that Thomas Hobbes's ideas about pneumatics were rightly rejected in favor of the superior knowledge advanced by Robert Boyle. But they gave no indication that it would be worthwhile to try developing Hobbes's ideas further. Historians, of course, have an easy answer here: it is not their job to develop scientific ideas actively. But whose job is it? It

is perfectly understandable that current specialist scientists would not want to be drawn into developing research programs that have been rejected long ago, because from their point of view those old research programs are, quite simply, *wrong*. This is where complementary science enters. Lacking an obligation to conform to the current orthodoxy, the complementary scientist is free to invest some time and energy in developing unorthodox systems.

Now I turn to one particular series of investigations that I have been making, in order to illustrate how these complementary-scientific developments might occur in chemistry. In the realm of chemistry, I think the easiest way into complementary work is through the recovery of lost knowledge from the past. Anyone who trawls through the primary literature of chemistry from before the 20th century will find reports of numerous facts that are no longer common knowledge among chemists, some of them even quite contrary to what we would expect today. Many such results are ripe for attempts at experimental confirmation by the complementary scientist, as the experiments involved tend to be relatively simple, cheap and easy to replicate.

the primary literature of chemistry from before the 20th century will find reports of numerous facts that are no longer common knowledge among chemists, some of them even quite contrary to what we would expect today. Many such results are ripe for attempts at experimental confirmation by the complementary scientist, as the experiments involved tend to be relatively simple, cheap and easy to replicate.

I started my experimental work in electrochemistry with the recovery of a phenomenon exhibited in an extremely simple and most intriguing experiment by the London physician-turned-chemist William Hyde Wollaston (1801, 427). He began with the well-known observation that certain metals dissolved in acids, releasing bubbles of hydrogen. This can be seen very easily by dipping a zinc wire in some dilute hydrochloric acid or sulphuric acid. If one inserts a silver wire into the same pot of acid, no visible reaction happens there since these acids do not attack silver. But just make the two wires touch, and hydrogen bubbles immediately start issuing from the silver as well as the zinc. Wollaston observed the same phenomenon with any combination of an acid and two metals, only one of which (on its own) is dissolved by the acid. I attempted replicating this experiment, and succeeded *immediately*. Could one imagine a simpler experiment? Yet, curiously, I have not met any chemists or chemistry students who had done this experiment before I showed it to them. It is an excellent case of a neglected piece of past scientific knowledge, very easily recovered.

Much else followed from my replication of the Wollaston experiment (see Chang 2011, sections 4–5, for a more detailed discussion). The difficulty of understanding what is going on in this experiment was as surprising as the ease with which it was reproduced. Wollaston's own view was that "in the solution of a metal, electricity is evolved during the action of the acid upon it"; the other (insoluble) metal "serves merely as a conductor of electricity, and thereby occasions the formation of hydrogen gas" at its surface (Wollaston 1801, 428–429). Wollaston was using the dominant conceptions of his day, which took electricity to be a fluid, and he favored the one-fluid theory. His theoretical account of the experiment, though very terse, was probably as good as any other story available at the time. For us today, however, it is not satisfactory to rest with Wollaston's account. By the recovery of Wollaston's experiment I have placed it in the twenty-first century, so it is no longer merely a piece of history; there is no compelling reason to stifle our scientific curiosity and refrain from seeking our own explanations of the phenomenon revealed in the experiment. Modern textbook accounts say that in an acid–metal reaction the hydrogen ions in the acid take electrons from the metal, turning into hydrogen gas; this transfer of electrons ionizes the metal, which then dissolves in the aqueous acid. But if that is what happens, how does the reaction generate any *excess* electrons that travel over to the silver side to make hydrogen gas there? In my opinion, this is an incomplete account of what acids and metals do to each other. Yes, according to the common Brønsted–Lowry theory of acids it is the hydrogen ion that defines acidity, and  $H^+$  concentration is indeed what pH meters measure. But it seems to me that a crucial role is also played by the anion (the negative ion), which is specific to each acid.

Things got even more interesting when I realized that the topology of Wollaston's experiment was actually the same as that of Volta's cell (which had just been announced a year earlier in 1800): namely, two different metals with an electrolyte between them. Indeed, Wollaston attempted to use his experiment in order to support an alternative theory of the Voltaic cell to Volta's own. Now, if Wollaston's set-up is Volta's cell, then we should be able to understand it simply by referring to the modern explanation of Volta's cell. So, what is the standard modern explanation of Volta's cell? Surprisingly, there isn't one readily available. Standard theoretical treatments of electrochemical cells in physical chemistry textbooks occur under the rubric of thermodynamic equilibrium, and they focus on computing the steady-state half-cell voltages from the Nernst equation (e.g., Atkins and De Paula 2010, chapter 6). For anyone wanting a rather mechanical or causal story about how free electrons start getting

produced and get moved about, the modern textbook theory is a difficult thing to apply. Most of the lower-level or practically oriented textbooks do attempt to give a more intuitive explanation of electrochemical cells, but in such texts what we get almost everywhere we turn is an explanation of the Daniell cell (named after the 19th-century London chemist John Frederic Daniell), in which the electrolyte consists of two different solutions connected by a salt bridge or a porous barrier (just one example out of a multitude is Housecroft and Constable 2010, 638). In this set-up each metal is dipped in its own solution, and the electrical activity is conveniently explained in terms of the imbalance of the redox potentials on the two sides. But Volta's original cell, which has only one electrolyte, containing no ions of either metal to begin with, cannot be explained in this way. Consequently Volta's cell has disappeared from basic electrochemical thinking; so has Volta's original theory, which attributed the electrical action to the contact between two different metals, not to chemical reactions. Volta's notion of contact action survives in the form of the physicist's contact potential (linked to the work function of each metal), but this is not part of the standard chemical discourse today.

The above line of thinking illustrates how recovery can effectively raise critical awareness. Realizing the difficulty of explaining Wollaston's experiment (and therefore the Voltaic cell) made me doubt that any of the available theories would have been straightforwardly superior to the others. This sense was enhanced strongly by some existing historiography that I then found. For instance, Helge Kragh (2000) concludes that the dispute between the Voltaic and the "chemical" theories of the battery continued throughout the 19th century, and fizzled out without a clear resolution. Kragh's survey is admittedly preliminary, and I intend to build on his work and other literature, including Wilhelm Ostwald's [1895] (1980) classic history of electrochemistry, to make a comprehensive and in-depth historical–philosophical–scientific study of this subject.

Enhanced critical awareness is something that I expect to reach in almost any investigations in the history and philosophy of science. Much less clearly anticipated when I first stepped into Wollaston's shoes was the possibility of *extending* the knowledge that I was recovering. The most interesting line of extension came from wishing to be more faithful to Volta's own experiments, in which he had used salt water, not an acid, as the electrolyte. I had concluded, as explained above, that the anions in the electrolyte must play an active role. In a zinc–copper Voltaic cell, the  $\text{Cl}^-$  ions attack the zinc, drawing  $\text{Zn}^{2+}$  ions into the solution and creating an excess of free electrons within the metal; these electrons then get pulled into the copper by the Voltaic contact force, and get released into the NaCl

solution from the copper side. But then what happens to these electrons? They seem to disappear without a trace. There is no production of hydrogen bubbles in this experiment, and all the chemists tell me that it is not imaginable that the electrons would combine with sodium ions ( $\text{Na}^+$ ) in the NaCl solution—and sure enough, there is no sodium metal produced at the copper wire. This puzzle led me to an extension which does not seem to have occurred to Volta and his contemporaries (though I may be wrong about this), while they certainly had the material resources for it: what happens if we pump *lots* of electrons into the NaCl solution, by connecting a battery into the circuit with the negative terminal connected to the copper? The result of this experiment is quite striking: on connecting the battery (initially I just used two commercial 1.5 V batteries in series), there is immediately a fizz of very active bubbling from the copper wire; meanwhile the copper wire also begins to darken and then becomes coated in a thick layer of black gunk. From the zinc side a white precipitate starts to come off. The theoretical analysis of what happens in this experiment is a rather long and ongoing story, but my provisional conclusion is the following. The gas coming out of the copper wire is hydrogen, the black deposit on that side is zinc, and the white precipitate coming from the zinc side is zinc hydroxide. As the number of  $\text{H}^+$  ions in an aqueous solution of NaCl is quite low, it must be the case that the battery is able to decompose water directly at the cathode (copper wire), creating  $\text{H}_2$  gas there and releasing  $(\text{OH})^-$  ions, which migrate over to the anode to combine with zinc there.

A most interesting experimental extension happened serendipitously when I attempted to make this experiment cleaner and simpler by eliminating chemical reactions going on at the anode, thinking that this would allow me to observe the cathode-side reaction with less interference. To this end I replaced the zinc wire constituting the anode with a gold wire. Contrary to my expectation (and that of all the chemists to whom I have shown this experiment so far), the gold wire began to dissolve immediately, producing a very visible yellow streak that flowed down freely and eventually produced a brown precipitate. I need to study this reaction and its products further. One interesting fact is that the solution of gold takes place only in a small window of applied voltage, roughly 2V–3V (at over 3V, chlorine gas is produced at the anode without a solution of the gold), the exact limits depending on the concentration of the salt. As for the concentration, initially I observed the phenomenon in a saturated solution, but subsequently discovered that concentrations of NaCl as low as 1/20 of saturation will allow the solution of gold. And having performed these experiments I then discovered at least one past



report of a similar phenomenon (Cruickshank 1800, 256), so now I also know that the same knowledge could have got at by recovery as well as by extension.

The above examples illustrate the kinds of benefits that can come from complementary science. I hope I have managed to illustrate clearly how complementary science can enhance our knowledge of nature, and also how it can enrich our historiographical engagement with past science. But it may not be obvious whether it has any relevance to the philosophy of chemistry as it is normally practiced (or the philosophy of science more generally), so I would like to consider that question more carefully here. I believe that each of the three categories of benefits of complementary science is highly relevant to the philosophy of chemistry. The obvious one is *critical awareness*, which should be part of the aim of almost any philosophical endeavor. Philosophers may try to create critical awareness out of nowhere, but it is much easier to do so by addressing once-live scientific questions that are no longer actively considered by most professional scientists. A prime example is the question about the extent to which chemistry has been reduced to quantum physics, which has been a staple topic of discussion in the philosophy of chemistry (e.g., Scerri 2008, Section A). Many other questions have been raised in a similar way by philosophers of chemistry, for instance about the nature of chemical bonds and the concept of the element. *Recovery* of lost scientific knowledge may not be seen as the business of philosophy as it is normally conceived. However, history can be a most effective critical–philosophical tool, to the extent that it displays alien systems of knowledge that can open up our minds about different conceptual possibilities and keep us from taking the current scientific orthodoxy for granted. Recovery of lost phenomena, as seen above in the electrochemical examples, has a wonderfully stimulating effect on theoretical and philosophical thinking. Similar liberating effects come from the recovery of lost ideas. Witness what it does to our metaphysical imagination, for example, to learn that there were many alternative forms of the periodic table, or that Lavoisier considered caloric a chemical substance liable to enter into chemical combination with other substances, or that Luigi Valentino Brugnatelli treated electricity as an acid. Finally, most philosophers would shrink from venturing into the realm of *extension*, and philosophers of chemists are no exception. But I think philosophers of chemistry would do well to take heed of extension, at least as a reminder of the actual fluidness of the seemingly fixed boundary between science and philosophy.

Before closing, I would like to try to articulate more clearly why chemistry seems to provide such fertile ground for complementary



science. There is something in the nature of chemistry, at least in its earlier phases up to the end of the 19th century but also in its underlying empirical foundations to this day, that encourages the participation of non-specialists. Most chemical experiments are not dry (in both senses of the word). They engage all five senses, and in ways that are stimulating to the uninitiated—the bright colors, the pungent smells, the strange tastes, the bangs of explosions large and small, and the varied textures. A wonderful sense of serious amateur delight is conveyed by the neurologist Oliver Sacks in his memoir *Uncle Tungsten* (2001), the feel of which is not so different from that of many chemical publications in the years around 1800. Chemistry is not too difficult to do like most of biology, and not too austere like much of school physics. A number of classic chemical topics are simple enough for most people to consider and experiment with (if sufficient health-and-safety precautions are taken), yet the phenomena and their explanations are complex enough to be intriguing. Moreover, the modern situation is that there are a number of *everyday* topics (ranging, in my own experience, from the physical chemistry of boiling water to the electrochemistry of the battery) that are not readily covered by today's textbook theories. That is to say, there is an abundance of phenomena in chemistry that are readily relevant to the public yet neglected in any level of modern science that they have access to. This makes very fertile ground for complementary science.

In many ways, complementary chemistry looks back to the golden age of amateur science around the year 1800. That is precisely the period during which my main illustrative case in this paper, early electrochemistry, originated and flourished. One key vehicle of early electrochemistry was William Nicholson's *Journal of Natural Philosophy, Chemistry, and the Arts*, founded in 1797. Historian Samuel Lilley has expressed a very apt admiration of what Nicholson achieved with his journal, which was to create a unique intellectual space for promoting what Lilley called "popular research": "The new movement was no mere passive desire to hear what had already been discovered. It was an extension to wider numbers of the desire to take some part in further discovery . . . many investigators whose names are now almost forgotten undertook researches and contributed each his small share to the sum of scientific knowledge." (Lilley 1948–50, 79) In the forum provided by Nicholson's *Journal*, and later also by competing periodicals such as Alexander Tilloch's *Philosophical Magazine* and Thomas Thomson's *Annals of Philosophy*, serious amateurs could converse at least occasionally at the same level with the few professional scientists that there were, and make some original contributions to the cutting edge of

science. The best showcase of popular research Lilley presents is the work in early electrochemistry stimulated by and reported in Nicholson's Journal, following its 1800 publication of the work by Anthony Carlisle and Nicholson himself on the first electrolysis of water by current electricity (*ibid.*, 83–89). Anybody armed with sufficient curiosity and determination, and a few bits of metal (such as coins) and a few other simple substances, could do research at home in this exciting field and hope to publish some discoveries or critical judgments.

The days of Nicholson are long past in science, and “popular research” has on the whole been swept decisively aside by the triumphant professional and specialist science of the 20th century. Yet, paradoxically, it is now the very success of specialist science that calls for a revival of popular research, no longer as part of the dominant frontier of science but as a necessary shadow of specialist science. And in our 21st century, with its deep and wide pockets of affluence and the participatory–democratic potential of the new electronic technologies, the conditions are ripe again for popular research, only with an even larger basis. Complementary science, with chemistry at its head, promises a decisive renewal of scientific knowledge for the many. It will give people an experience of genuinely open-ended inquiry, which will generate a lively appreciation of the relevance of science for everyday life, and of scientific methods as they are actually practiced. Such experience will also foster intellectual humility in the face of the abundance of nature, and along with it a well-grounded and critical appreciation and respect for specialist science and its achievements.

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# **TRANSCENDENTAL APPROACHES**

# A KANTIAN PERSPECTIVE FOR THE PHILOSOPHY OF CHEMISTRY

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## Introduction

When compared with other areas of the philosophy of science, the philosophy of chemistry is a new branch that entered an already highly developed field of research about science. For this reason, in spite of having opened its own agenda, the philosophy of chemistry inherited a style of philosophizing modeled by the post-positivistic analytic tradition. Although one cannot deny the powerful conceptual tools that this tradition offered to the philosophy of science of the twentieth century, one can neither ignore the strong boundaries that it imposed to what can be thought in the field. One of the areas that remained beyond those boundaries was the Kantian philosophy. In fact, the debates about scientific realism were usually confined to the non-observational domain, whereas the existence of a realm of observable entities independent of any knowledge was acritically accepted by the traditional philosophy of science. And although the “new philosophy of science” began to challenge that strongly entrenched assumption, the analytic tradition rapidly drove the discussions to the domain of language. As a consequence, the problem of realism in science is still analyzed by many authors in terms of the search of a theory of reference for the scientific language, a strategy that confines the debate to a context where the analytic philosophers feel comfortable.

The general purpose of this article is to contribute to broaden the perspective of the contemporary philosophy of science by taking seriously the Copernican revolution proposed by Kant, which places the subject at the center of any research about knowledge. We will argue that Kantian ideas supply a new perspective to face several of the most discussed topics in the philosophy of chemistry, in particular, the relationship between chemistry and physics, as well as the existence of laws in chemistry and the question about chemical kinds.

## 1. Chemistry and Physics

Although chemistry evolved independently of physics, in the history of the discipline there were certain attempts to explain chemistry in mechanical terms. This was the case of Bernard le Bovier de Fontenelle, perpetual secretary of the French Academy of Sciences, for whom chemical phenomena should be explained in terms of atoms with no other properties than geometric ones (the debate between Fontenelle and Vernel on this topic, in the mid of the eighteenth century, is reported by Bensaude-Vincent and Simon 2008). However, it was only since the impressive success of quantum mechanics that the idea that chemistry can be completely reduced to physics pervaded the scientific community (recall Dirac's famous dictum, 1929, p. 714). In other words, chemistry began to be conceived as a branch of physics to the extent that it deals with complex systems or particular processes which, nevertheless, could 'in principle' be described and explained by means of quantum theory. This assumption not only deprives the philosophy of chemistry of legitimacy as a field of philosophical inquiry, but also counts against the autonomy of chemistry as a scientific discipline: whereas physics turns out to be a "fundamental" science that describes reality in its deepest aspects, chemistry is conceived as a mere "phenomenological" science, that only describes phenomena as they appear to us.

In recent years many philosophers of chemistry have begun to challenge that traditional assumption in order to recover the autonomy of chemistry and, as a consequence, the legitimacy of the philosophy of chemistry. The autonomy of chemistry is usually defended on the basis of the failure of epistemological reduction: not all chemical concepts and laws can be derived from physics. In particular, many relevant chemical notions, as chemical bond, chirality, molecular shape or orbital, among others, are not amenable to rigorous quantum mechanical treatment. For instance, Vemulapalli and Byerly (1999) claim that epistemological reduction fails even in relatively simple cases, since the properties of a chemical macro-system can never be derived from its micro-components without additional assumptions of chemical data. In a similar sense, Scerri and McIntyre (1997) argue for the need of eschewing the epistemological reduction of chemistry to physics.

In spite of this agreement among the philosophers of chemistry about the epistemological autonomy of chemistry, in the relationship between chemistry and physics ontological reduction is usually taken for granted: chemical entities are, when analyzed in depth, nothing else than physical entities. The implicit idea is that the impossibility of epistemological

reduction is only due to technical difficulties, derived from the enormous complexity of the chemical systems, but not to the fact that chemistry refers to its own ontological domain (for explicit claims in this sense, see Benfey 2000; Luisi 2002). This perspective guarantees the methodological autonomy of chemistry with respect to physics, since it provides chemistry with a realm of specific concepts that have no place in fundamental physics. However, the mere failure of epistemological reduction is not sufficient for rejecting the secondary position of chemistry with respect to physics. When the ontological reduction of the chemical world is not questioned, the fundamental physical realm has ontological priority; chemical descriptions only refer to appearances or, at most, to secondary entities endowed with a merely derived existence. In other words, whereas physical descriptions would refer to the true and ultimate ontology, the “noumenal” realm, chemistry would only describe an ontologically inferior level of reality, a “merely phenomenal” domain. In turn, this metaphysical view has significant implications for the philosophy of chemistry itself: if chemical entities are no more than secondary entities ontologically derived from the underlying physical domain, the philosophical problems of chemistry, when considered in depth, are problems belonging to the philosophy of physics.

In the last decade some attempts have been directed at reversing the secondary position of chemistry by appealing to symmetrical relations between the discourses of chemistry and physics (van Brakel 2000a, b) or to autonomous though related levels of reality (Scerri 2000a, b). It is precisely at this point that a Kantian rooted perspective offers a well-articulated philosophical framework for supporting the ontological autonomy of the chemical world (Lombardi and Labarca 2005, 2006).

According to Kant, the reality independent of the subject is a noumenal realm, which is not object of our knowledge. It is nonsense to think about an independent ontology, since there are no objects in the noumenal reality: the noumenon is ineffable; it can only be conceived as a limit of thought. The ontology, inhabited by the objects of knowledge, results from the synthesis between the categories of the understanding and the material coming from the experience: thoughts without content are empty, intuitions without concepts are blind (Kant 1781, p. A 51, B 75; in the original German: “*Gedanken ohne Inhalt sind leer, Anschauungen ohne Begriffe sind blind*”). Therefore, the world to which our scientific knowledge refers is not a mere “epistemologized” ontology resulting from our contingent means of access to reality, in the same sense as the Kantian system is not an epistemology but a broad philosophical framework that

establishes the necessary conditions of possibility for knowledge and, therefore, for any meaningful scientific discourse.

After having adopted a precritical realism for years, in his book *Reason, Truth and History* Hilary Putnam (1981) defends an explicitly Kantian rooted ‘*internalism*’ or ‘*internalist realism*’, as contrasted with externalism or metaphysical realism, also referred to as “God’s eye point of view”. According to externalism, the world exists independently of our knowledge, and consists of some fixed totality of subject-independent objects. Then, there is only one true and complete description of ‘the way the world is’. By supposing that reference is a relationship between the words of the language and the external, independent ontology, externalism needs a non-human point of view –God’s eye– to fix the reference of the language and, with this, the truth-value of its sentences: scientific realists “speak persistently of the reality of the external world, as if they were disembodied spirits contemplating it from the outside, and, for all their godlessness, they put forward a view of it that is only conceivable from the standpoint of an omniscient God.” (Torretti 2000, p. 114) From this perspective, science reveals the only “true” ontology, since its propositions mirror the “ready-made” world.

For the internalist, on the contrary, “«objects» do not exist independently of conceptual schemes. We cut up the world into objects when we introduce one or another scheme of description” (Putnam 1981, p. 52). The question ‘What objects does the world consist of?’ only makes sense to be asked within a theory or description. This means that conceptual schemes are not mere intermediary between subjects and objects; rather, they play an essential role in the constitution of objects. Therefore, even though there is a noumenal reality independent of the subject, the ontology only arises from the synthesis between that noumenal reality and a conceptual scheme. Objectivity does not mean independence from the subject, but it results from that synthesis. Thus, science does not reveal an independent reality, but participates in the constitution of its ontology.

However, as Torretti claims, Kant’s “conception of the understanding as a closed system of rules with full authority over every cognitive judgment makes it virtually impossible to think that there is more than one form of understanding, expressed in a single fixed «categorical framework» or «conceptual scheme»”. (Torretti 2008, p. 87) But the explosive growth of knowledge in the last two centuries has persuaded us that the very idea of intellectual closure cannot be seriously defended. For this reason, Putnam admits the possibility of multiple conceptual schemes, irreducible to each other, and this leads him to the thesis of *ontological pluralism*, according to which each successful conceptual scheme constitutes its own



ontology. Ontological pluralism has been widely discussed in the context of the problem of theory change, where it has been appealed to for rejecting the scientific externalism that assumes the convergence of science towards the true description of the real ontology –the One True Theory–. Nevertheless, when we realize that different theories –and even different disciplines– are accepted at the same historical time and in the context of a single paradigm, we must also infer that different ontologies may coexist since each one of them is constituted by its corresponding conceptual scheme. Since the privileged viewpoint of God’s eye does not exist, there is not a single “true world”: all the ontologies coming from successful science have the same status, and all of them are constituted by equally objective descriptions. It is from this viewpoint that the multiple and different scientific practices become intelligible.

The philosophical framework supplied by a Kantian-rooted thought is particularly relevant for addressing the relationship between chemistry and physics. From this perspective we can realize that the traditional assumption of ontological reduction is implicitly based on a metaphysical realism, according to which there exists a single ontology: all the objects, properties and regularities not belonging to it have a “secondary” existence, which depends on–and, then, can be ontologically reduced to–the fundamental items of the only real world. From this perspective, emergence is merely epistemic. In particular, the ontological priority of the world of physics is taken for granted and, as a consequence, physics is supposed to describe reality as it is in itself. Chemistry, on the contrary, is conceived as referring to an ontologically secondary realm, inhabited by entities and properties that have only a derived existence. Therefore, the intertheoretical relations that can be successfully established between chemistry and physics are viewed as mere definitions or contingent conditions, which do not add nomological content to the theoretical descriptions given by physics. As a consequence, the discourse of chemistry is only an economic way of saying what we could have said, in principle, with the discourse of physics.

This precritical view can be rejected from a synchronic ontological pluralism. In fact, when the idea of God’s point of view is given up, it is not yet possible to conceive the description of reality in itself: even quantum theory corresponds to a particular conceptual scheme that constitutes the quantum ontology. On the other hand, chemistry involves its own conceptual framework and, as a consequence, refers to its own ontology. If chemical concepts could be epistemologically reduced to quantum concepts, there would be a good reason to believe in the ontological reduction of the chemical world to the ontology of quantum

mechanics (see Labarca and Lombardi 2010, Lombardi and Castagnino 2010). But when the limits of the epistemological reduction of chemistry are recognized, there is no argument other than a precritical metaphysical realism for postulating ontological reduction.

Summing up, from this Kantian rooted perspective, chemical concepts, like composition, chemical bonding, chemical reactivity, molecular shape and orbital, refer to entities belonging to the chemical ontology, which only depends on the theory that *constitutes* it and does not derive from an ontologically more fundamental level of reality. Therefore, successful intertheoretic relations between chemistry and physics should not be interpreted as definitions or contingent conditions, which manifest an asymmetric dependence between a merely phenomenological realm and the fundamental reality. On the contrary, those relations have to be viewed as intertheoretic laws, which express a nomological symmetric relation between two autonomous ontologies. This means that intertheoretic relations are not “stairs” between different levels of objectivity, but “bridges” that link equally objective ontologies and that can be crossed in both directions. In this way, the Kantian inspired internalism supplies a philosophical framework that allows us to face the problem of the relationship between chemistry and physics, without confining the chemical world to an apparent or secondary realm.

## 2. Laws of Nature and Natural Kinds

A relevant question addressed by the contemporary philosophers of chemistry is that referred to the existence of chemical laws. For some authors, laws are the mark of scientificity and, therefore, the laws of chemistry are natural laws to the same extent as the laws of physics. In particular, Mendeleev’s periodic table is conceived as a law, with an appeal to idealization in the same sense as in the case of physical laws (see, for instance, Hettema and Kuipers 1988; Vihalemm 2003). Other authors, on the contrary, consider that a significant part of chemistry is based on mere classifications with no nomological content. In this sense, Eric Scerri (1997) claims that the periodic table itself is neither a theory nor a law: it is a way of representing a periodic system, which is devoid of theoretical status since its only purpose is classification but not explanation.

The disagreement about chemical laws shows that a problem strongly linked with the general question about laws is that referred to the existence and definition of natural kinds. In fact, natural kinds are precisely those kinds to which scientific laws intend to apply. In other words, science studies certain kinds supposedly resulting from a grouping that does not

depend on humans. Although cases of those kinds may be found in all disciplines, at present chemistry has replaced biology in providing paradigm examples of natural kinds: chemical elements and chemical compounds. The central question in this context is: are putative natural kinds genuinely natural or merely conventional? In the chemical context, the question about the existence of natural kinds has been strongly linked with the assessment of microstructuralism, according to which chemical kinds can be individuated solely in terms of their microstructure (see van Brakel 2000a; Needham 2002; Hendry 2006).

The debate about the nature of the laws of nature and of natural kinds has been marked by two extreme views: conventionalism (or psychologism) and essentialism. According to the first, Humean-style position, laws of nature are mere summaries of experiences, with no natural necessity, and natural kinds are conventional groupings that do not carve nature at its joints. Conventionalists may accept that science employ certain kinds, but they conceive that particular selection as a mere convenient decision that depends on particular purposes, and that can be replaced when the purposes change. On the opposite side, essentialism conceives a natural kind as demarcated by a real essence, that is, what makes an individual to belong to that natural kind and not to another. From this perspective, laws of nature are statements that express real and necessary relations between essences.

Under the strong influence of empiricism –as that of Mach (1890), which modeled the thought of the Vienna Circle– the philosophy of science of the first half of the twentieth century adopted positions closer to Humean views than to essentialism. Nevertheless, those views cannot justify why laws may legitimately be extrapolated from what has been observed to what has not happened yet, that is, they cannot account for the possibility of scientific predictions. In turn, since laws are conceived as summaries of what did happen, is happening, and will happen, real possibilities simply do not exist in the world of the strong empiricist. As a consequence, this perspective has no means to account for the fact that genuine laws support counterfactuals, while mere accidental generalizations do not (Goodman 1965).

Perhaps for those difficulties, but also thanks to the decline of the logical-positivistic influence, essentialism experienced a revival during the 70s and the beginnings of the 80s, mainly in regard to natural kinds. The works of Kripke (1972, 1980) and Putnam (1973, 1975) addressed the question from a semantic view: by extending the causal theory of reference for proper names, Kripke and Putnam considered that natural kind terms refer directly to the members of the kind; in turn, each kind is

demarcated by its essence, which is discovered by science. Since there is a close relation between what is taken as a law of nature and what is recognized as a natural kind, essentialism about natural kinds has immediate implications for the way the laws of nature are understood. For instance, if essences are conceived as universals, natural laws can be viewed as relations holding between universals (Dretske 1977; Tooley 1977; Armstrong 1978, 1983). According to some authors, those universals are powers, tendencies or dispositions (see Bhaskar 1975; Harré and Madden 1977): the world is populated by a multiplicity of natural dispositions, which tell us the possibilities inherent in the natures of things, and what kind of thing we are dealing with is itself specified by the dispositions that define it (Harré 2000). Of course, an essentialist perspective is the best antidote against the shortcomings of Humean-style views, though at the cost of turning science into metaphysics. Moreover, essentialism also has to face difficulties, in particular when applied to real-life science. For instance, according to Dupré (1993), contemporary scientific understanding of biological species lends little support to essentialism (see also Hull 1965) and, as a consequence, he stresses the need of a variety of more or less cross-cutting classificatory systems (Dupré 2000; the same situation has been pointed out for chemistry in Llored 2012).

The supposedly dichotomic alternative between essentialism and conventionalism is stuck at the heart of chemistry. In fact, the paradigmatic example in the arguments of Kripke and Putnam is “water is  $\text{H}_2\text{O}$ ”. Essentialism in chemistry takes the form of microstructuralism. This approach seems to work for chemical elements, since the atomic number suffices to identify the element. However, when microstructuralism is extended from elements to compounds, difficulties begin. In fact, the identification of a compound only by its composing elements is seriously challenged by isomerism, since molecules of isomers have the same atoms spatially arranged in different ways. Moreover, Needham (2000) has argued that compounds as water may have a dynamical structure that cannot be adequately described by their chemical composition formulas. Hendry (2006) takes the argument a step further when he stresses that any sample of liquid water, even if pure, contains not only  $\text{H}_2\text{O}$  molecules, but also  $\text{H}_3\text{O}^+$  and  $\text{HO}^-$  ions. Things get worse for microstructuralism when we search for classifications of elements according to their macroscopic properties: even when we are able to establish connections between the two levels of description, the possession of a microstructure does not imply the display of any characteristic chemical behavior at the macrolevel. In fact, the particular electronic configuration of an element

does not fix its macro-properties (see Scerri 1997): for instance, although helium, beryllium and magnesium have the same outer shell configuration, helium is a highly inert gas while beryllium and magnesium are reactive metals. Moreover, due to the phenomenon of allotropy, different instances of a single element may fall in different categories.

Of course, these difficulties of essentialism in chemistry do not lead us to embrace the opposite, Humean-style view, since it would let us with no justification of the high practical success of the classifications and the laws of chemistry. Some authors have tried to find an intermediate position by proposing a kind of pluralistic stance that avoids the problems of both extreme views: the central idea is to acknowledge that science may require a variety of more or less cross-cutting classifications. For instance, Dupré (1993) defends a “promiscuous realism”, which does not renounce the use of the term “natural kind”, though clearly in a sense stripped of its traditional essentialist connotations. A similar perspective is adopted by van Brakel, when he claims that “we could be tolerant enough to leave equal *ontological* room for manifest water, water in terms of the thermodynamic theory of substances, the molecular structure of water (‘constructed’ out of spectroscopic measurements), the ‘proper’ quantum mechanical equations for an isolated water molecule, and experiments with isolated water molecules which, depending on the measurement technique, show more or less of the ‘classical’ molecular structure” (van Brakel 2000b, pp. 147-148).

At this point it is worth noticing that, in the attempts to avoid both the Scylla of conventionalism and the Charybdis of essentialism, the Kantian philosophy is not even mentioned. The traditional debate about laws of nature and natural kinds proceeds from an “externalist” perspective, as if we could adopt God’s eye position to decide what exists and what does not exist in the world. This situation is framed in the general trend followed by the twentieth century analytic thought: in the context of this philosophical framework, problems have been usually addressed from precritical stances, as if the turning point introduced by Kant in the Western philosophy had not even existed. However, once one retrieves the teachings of Kant about the constituted nature of the world of knowledge, the discussion appears in a new light, and pluralistic views acquire a philosophical foundation.

In fact, from a Kantian-rooted ontological pluralism we can accept the existence of legitimate laws of nature and natural kinds in each ontology constituted by a successful conceptual scheme: those laws are not mere summaries of experiences, and those kinds are not conventional groupings without any reference in the world. Nevertheless, this does not lead us to

adopt a metaphysical essentialism, committed with absolute laws of nature and with natural kinds populating reality in itself. The active role played by the subject in knowledge is what supports the fact that laws of nature and natural kinds result from the synthesis between the noumenal reality and a conceptual framework expressed by a discourse that is the verbal manifestation of a successful scientific practice. And, in turn, the possibility of multiple conceptual schemes, derived from different successful practices, opens the way for different but not reducible laws and multiple cross-cutting classifications, all of them equally natural and objective, although not essential. Their objective nature relies not on the fact that they mirror reality as it is, independently of the knowing subject, but on the scientific activity as a productive praxis. From this pragmatic viewpoint, chemistry certainly holds the winning card: its astonishing achievements in the manipulation of known substances and in the production of new substances and materials are the best reason for accepting its laws and kinds as proposed in its different subdisciplines.

## Conclusion

After a hardly justifiable omission of the Kantian thought in certain domains of the philosophy of the twentieth century, the present paper aims at recovering a central role for criticism in the philosophy of chemistry in particular and in the philosophy of science in general. From the perspective of a Kantian rooted ontological pluralism, we have argued for the ontological autonomy of the chemical ontology, and against views that turn the world of chemistry into a merely “apparent” or “derived” domain, with a secondary status with respect to the “primary” world of “fundamental” physics. On the other hand, we have proposed that perspective as the philosophical framework that supplies the foundations for an intermediate position between conventionalism and essentialism in the traditional debate about the nature of the laws and kinds involved in science, a debate particularly active in the philosophy of chemistry.

Of course, our position will be certainly unacceptable for the analytic philosopher, whose thought closely linked to the words of a language prevents him to reach the world of things. But our perspective may also be criticized by the scholar devoted to the study of the Kantian corpus, who might say that we are not truly Kantian because we accept an ontological pluralism that relies on a multiplicity of categorial frameworks. This is a debate in which we are not interested to be engaged. Our purpose has been to support the idea that the ontology of our knowledge is not independent of our categorial frameworks: this idea, whose Kantian origin cannot be

denied, supplies a philosophical background to successfully address many problems in the vigorous field of the philosophy of chemistry.

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# PRAGMATICALLY NATURALIZED TRANSCENDENTAL PHILOSOPHY OF SCIENCE AND PHILOSOPHY OF CHEMISTRY

SAMI PIHLSTRÖM

## Introduction

Philosophy of science has over the past couple of decades—following successful interdisciplinary inquiries in science and technology studies, in particular—taken the concrete *local practices* of historically contextualized scientific inquiry much more seriously than more traditional philosophies of science, such as logical empiricism and its follow-ups, including standard versions of scientific realism and neo-Kantian social constructivism, ever did. Attempts to understand the nature of science have thus shifted from “global” questions of justification, for example concerns with the logical structure of scientific theories, scientific inference, and scientific explanation—concerns arguably culminating in what may be regarded as “transcendental” issues concerning the very possibility of cognitive experience or scientific knowledge and representation—to more “local” issues of, say, modeling and other epistemic activities whose central cognitive goals and strategies are strongly practice-embedded and even unintelligible without a practical context. These changes concern the philosophy of chemistry as much as any other special field within the philosophy of science. Indeed, research in special fields like philosophy of chemistry has presumably been considerably intensified as a result of the “local turn”.

This shift, though understandably resisted by traditional philosophers of science fearing the excesses of relativism, is in many ways a welcome one. However, it is very important to realize that the shift from the global to the local is *not* inevitably a move to a completely non-transcendental approach to science. By developing this point I will, in the following, also argue, at a more general level, for the compatibility and even the mutually enriching potential of the pragmatic and the transcendental perspectives on

science. While my explicit comments on philosophical issues in chemistry will be scarce, my general discussion of “naturalizing the transcendental” in the philosophy of science should, I believe, be of interest to those working that field, too.

## 1. The Pragmatic and the Transcendental

I want to begin by arguing that taking local scientific practices seriously does not automatically mean that one is a resolutely non-Kantian philosopher in one’s account of scientific inquiry. This is because the Kantian or quasi-Kantian “transcendental” element—whatever it is that must be presupposed for inquiry, representation, or cognition to be possible—may lie in the local practices themselves.<sup>1</sup> This is an insight that may be developed through a Kantian reading of Thomas Kuhn’s work, in particular. Kuhn, after all, was a major figure—perhaps the most important figure—behind the “practice turn” of contemporary philosophy of science and science and technology studies. (Cf. Kuhn, 1970, 2000; see also Pihlström & Siitonen, 2005)

According to Kuhn’s well-known statement, the notion of truth, insofar as it has anything to do with the developments of science and scientific theories, cannot be “extra-theoretical” correspondence but must instead be understood “intra-theoretically” (Kuhn, 2000, pp. 115, 160-162, 251). This does not mean any naïve anti-realism or constructivism, however. There is a sense in which the world is “experientially given” and “solid”, instead of being something that we (or the scientists) simply “make up” (ibid., p. 101). Even in Kuhn’s late work, there is, nevertheless, a version of the famous idea of different paradigms’ constituting “different worlds” (cf. Kuhn, 1970, pp. 111, 206): he does speak about the “world-constitutive” role of human intentionality and mental representations (Kuhn, 2000, p. 103). The world *is* in some sense constituted or structured, if not literally constructed, by the human mind—or, more specifically, by scientific theorization and other epistemic activities, both strictly scientific and more loosely everyday ones.

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<sup>1</sup> Generally, Kantian transcendental philosophy—following Kant’s (1781/1787) discussion of the necessary conditions for the possibility of cognitive experience—engages in inquiries into necessary conditions for the possibility of certain given human actualities, such as (in addition to experience, Kant’s main concern) linguistic meaning (Wittgenstein) or scientific representation. It is always controversial to read later thinkers as “Kantian” or “transcendental”; my suggestions in this regard must therefore be regarded as provisional and suggestive rather than aiming at historical accuracy.

In this way, Kuhn does seem to argue, early and late, that local scientific practices *are* in the business of world-constitution. Indeed, the plausibility of the Kuhnian view of the world-constitutivity of paradigms and intra-theoretical truth seems to depend on the availability of a Kantian interpretation and/or reconstruction of Kuhn's occasionally more than just mildly obscure statements. Kuhn himself admitted in his late work that he had developed "a sort of post-Darwinian Kantianism", with "the lexicon" supplying "preconditions of possible experience" in a way analogous to the Kantian categories, yet differing from the latter by being relative to both time and community (ibid., p. 104). Kuhn should, then, be read as a Kantian with "movable categories" (ibid., p. 264) and without any permanently existing things in themselves (see ibid., p. 207); his "structured lexicon" and Kant's "a priori" may both, in a relativized sense, be taken to be "constitutive of *possible experience* of the world" without assuming that they could dictate what that experience must be in any concrete case (ibid., p. 245).

Yet, again, something analogous to the Kantian thing in itself must be at work even in Kuhn's system, because "something permanent, fixed, and stable" must be what underlies the changes of lexical categories (ibid., p. 104); anomalies requiring readjustments in scientific theories and paradigms could hardly occur at all, if everything there is were simply dependent on or constructed by us. There is, then, a curious combination of realism and idealism (constructivism) to be found in Kuhn—at least as profoundly as there is such a combination in Kant himself, who famously sought to integrate *transcendental idealism* with *empirical realism* and to avoid both dogmatic *transcendental realism* and skeptical *empirical idealism*. While the Kuhnian philosopher of science clearly need not employ this Kantian terminology, something like a Kantian vocabulary does seem to be required to make sense of the basic idea of the world being both ("transcendentally") dependent on scientific practices and ("empirically") independent of them; without a Kantian background this hardly makes sense at all.<sup>2</sup>

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<sup>2</sup> For more comprehensive discussions of Kuhn's relation to realism, constructivism, and Kantianism, see, e.g., Hoyningen-Huene, 1993; Andersen, 2001; Friedman, 2001, 2002, 2003; and Sharrock and Read, 2002. Nothing in my elaborations in this paper depends on getting Kuhn historically right; in particular, I do not want to take any final stand on the question of whether Kuhn offers novel ideas in the realism debate or leads us out of that debate. (Generally, I believe it is significantly harder to move out of that debate than some philosophers, including some Kuhnians, may think.) In addition to the Kantian interpretation defended by Hoyningen-Huene, in particular, it is important to note that Ian Hacking (1983)

Hence, we can now reach a conditional conclusion: *if* we want to make sense of Kuhn's view that the way the world is paradigm-relative (captured in the slogan that "the world changes" in a scientific revolution), or the related view that local practices of inquiry play a constitutive role in the emergence of scientific truths, facts, and objects, we should understand the relevant notions of paradigm-relativity and constitutivity in a (quasi-) Kantian transcendental sense, analogously to the way in which the objects of possible experience are, according to Kant himself, constituted by the categories (that is, the pure concepts of the understanding) and the forms of intuition.

## 2. Kuhn and Pragmatism

A key observation at this point is that the kind of Kantian reading of Kuhn sketched in the previous section is *not* inevitably non-pragmatist. We may, in a broad sense, understand both Kuhn's account of scientific paradigms and the more general practice-oriented conception of science in contemporary philosophy of science and science and technology studies as "pragmatist" in a broad sense. However, pragmatism can be a transcendental approach, too, as soon as we realize that the contextually necessary transcendental conditions for the possibility of cognitive experience (or, better, scientific representation of objective reality) are themselves practice-laden and historically revisable. While the classical pragmatists—Charles S. Peirce, William James, John Dewey, and others—were often highly critical of Kant (just think of James's pronouncement that the path of philosophical progress should be seen as moving from the

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proposes a "nominalist" interpretation, maintaining that the world that remains fixed and unchanging is a world of individuals, while the lexical categories defining a "world of classes [of individuals]" change in a paradigm shift. (Hacking, in the same book, also suggests that Hilary Putnam's "internal realism" can be understood as "transcendental nominalism".) Whether or not one sympathizes with a Kantian reading of Kuhn—comparing the unchanging element to the things in themselves—or perhaps, rather, Hacking's nominalistic reading—finding individual entities unchanging—one must in some sense specify what actually changes and what remains unchanged in scientific revolutions. As this is not a study on Kuhn in particular, I must leave such questions open. I am reluctant to make any firm commitments to there being any specific metaphysical element (e.g., things in themselves, individuals, or whatever) that is what it is "in itself" independently of paradigms and their changes, even though I am also reluctant to simply join anti-realist Kuhnians in suggesting that everything changes when a new paradigm emerges. I hope my comparison between Kuhn and pragmatism will help to clarify the need for such a middle ground position.

British empiricists “round Kant”, instead of “through Kant”, to pragmatism), this is in my view partly based on their possibly somewhat limited self-understanding, as well as their limited understanding of what has proven to be most important and sustainable in Kantian philosophy (see, e.g., Pihlström, 2003, 2008, 2009).

No obvious historical lines of influence can be traced from the classical pragmatists to Kuhn. However, Kuhn can, arguably, be interpreted—and has been interpreted by Michael Friedman and others—as joining, either explicitly or implicitly, if not those older pragmatists’ views, at least the quasi-pragmatist ideas later made famous by thinkers like Ludwig Wittgenstein and C.I. Lewis (as well as, possibly, Michel Foucault) concerning the *historically relative “a priori”*. Kuhnian paradigms (or lexicons) play this reconceptualized a priori role as *enabling* (making possible) scientific representation, and thereby also enabling scientific objects and truths to emerge from scientific practices and theorizing. By synthesizing Kantian and pragmatist insights, Kuhn’s position can be generalized into a more comprehensive version of historicized and naturalized (“pragmatized”) transcendental idealism and transcendental philosophy of science. (Cf. Pihlström, 2003, 2004; Pihlström & Siitonen, 2005.) Pragmatists more generally should be read as Kantian philosophers in the sense that they also challenged and continue to challenge transcendental realism, the supposition that the world possesses its “own” categorial ontological structure that our schemes and theories, or our science, can be expected to “cut at its joints”, i.e., to simply reveal (or to fall short of revealing) “as it is in itself” and that could at least in principle be accurately represented in an absolute theory (and cannot be so represented if we lack an absolute theory).<sup>3</sup>

It is extremely important to give up the apodicticity, unrevisability, and universality of Kantian transcendental principles, in order to re-entangle Kantianism and pragmatism in a way that preserves the constitutive function of those principles. As Friedman (2001, p. 30) explains, these principles need not be unrevisable in order to remain “constitutive of the concept of the object of knowledge”. One of the most important versions of this “relative a priori” is Lewis’s (1923) theory of the “pragmatic a priori” (cf. Järvillehto, 2011). Its relations to Kuhn’s ideas would deserve closer historical and systematic scrutiny—as would, obviously, Kuhn’s discussions of the development of chemistry in particular with regard to the historical changes of relative a priori assumptions.

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<sup>3</sup> The modern version of this view, already rejected by Kant, would be “metaphysical realism”, firmly rejected by Hilary Putnam and his many followers in the contemporary realism debate. See, e.g., Putnam, 1981, 1990.

This is not the right place to continue scholarly debates on what pragmatism actually means, either historically or systematically (see, e.g., Pihlström, 2011a); nor am I in this paper willing to return to the question of how exactly to write the history of pragmatist philosophy of science—assuming that there even is such a history to be coherently written (cf. Pihlström, 2008). Clearly, it is not necessary to adopt the concept of pragmatism at all in one's interpretations of either Kuhn or the practice-oriented philosophy of science more generally. Perhaps the label “pragmatism” in the end adds very little to the key idea of focusing on scientific practices. Nevertheless, it does seem to me that the ways in which the realism debate, in particular, have been continued in the pragmatist tradition—and carried on and transformed into a pragmatic shape from the Kantian transcendental tradition—offer illuminating comparisons to Kuhn and many post-Kuhnian philosophers of science who have taken the “practice turn”.

Joseph Rouse (2003) is one of the interpreters of Kuhn insightfully drawing due attention to Kuhn's role in emphasizing science as a practice. Rouse takes this to mean that Kuhn rejected the traditional epistemological questions of justifying scientific beliefs. However, while it is certainly correct to note that the traditional issue of epistemic justification is not central in Kuhn, this seems to presuppose an *unpragmatic* dichotomy between practices and beliefs, whereas the more obviously pragmatist response to the traditional questions of justification would be the insistence that beliefs *are* practices—or, as the classical pragmatists themselves often put it, “habits of action”. The view that beliefs are habits of action is one of the fundamental ideas of pragmatism all the way from the initiation of the pragmatist tradition by Charles S. Peirce and William James: beliefs are something on the basis of which we are prepared to act.<sup>4</sup> Thus, it is somewhat problematic that, after perceptively pointing out that Kuhn leads us to a shift toward a description of science as an *activity* (rather than as a *product* of an activity), Rouse continues to claim that paradigms ought to be understood as “exemplary ways of conceptualizing and intervening in particular situations”, *instead of* being understood “as beliefs (even tacit beliefs) agreed upon by community members” (ibid., p. 107).

From a pragmatist point of view, we may and should say that it is precisely in virtue of their being “ways of conceptualizing and intervening” that paradigms are *also* beliefs, or networks of beliefs—or perhaps “webs of

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<sup>4</sup> For Peirce, in particular, this was a methodological principle quite literally emerging from his experience in research laboratories—which is something that philosophers of chemistry, in particular, should be able to appreciate.

beliefs”, to employ a Quinean phrase (cf. section 4 below). It is in our goal-directed activities and practices themselves that our ontological ways of taking the world to be in some particular manner are to be located. There are, and can be, no beliefs at all apart from such activities and practices. Beliefs are inevitably based on practical contexts of inquiry, as the very purpose of inquiry is the fixation of belief, or the settlement of a problematic situation, and what this pragmatically involves is the acquisition of a new habit, or a revision of an already established one. Rouse’s dichotomies between “practitioners” and “believers” and between “beliefs and forms of life” (ibid., pp. 109, 112) are, then, simply too unpragmatic to be helpful in the context of my “transcendentally pragmatist” re-reading of Kuhn (and Kuhnian philosophy of science generally). Scientists, pragmatically speaking, are *both* practitioners *and* (hence) “believers”.<sup>5</sup>

### 3. Pragmatism as Naturalized Transcendental Philosophy: Holism and Interdisciplinarity

Pragmatism can, then, be rearticulated as a form of naturalized transcendental philosophy, both generally and in the context of contemporary philosophy of science, in particular. (And Kuhn himself, arguably, was a kind of pragmatist in this sense.) A further interesting analogy, drawn more directly from within the pragmatist tradition, could also be suggested here: Morton White’s (1956, 1986, 2002) *holistic pragmatism* can be seen as a version of the kind of pragmatically naturalized and historicized transcendental philosophy of science that the “local practices” approach in the philosophy of science today could utilize (although White himself might not be entirely satisfied with this characterization). Historical and systematic comparisons between Kuhn and White should be encouraged; very little work has so far been done in this regard. Kuhnian paradigms could be seen as practice-embedded sets of factual and normative assumptions governing inquiry in a given discipline or field, along the lines of White’s holistic pragmatism.

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<sup>5</sup> Accordingly, while Rouse’s reflections are generally very helpful in integrating (pragmatic) naturalism with irreducible normativity within scientific practices (see also Rouse, 2002), he offers no adequate historical treatment of pragmatism (which, of course, is not to say that he would have to do so...). As a matter of fact, I suggested already some time ago (see Pihlström, 1998, chapter 9) that Rouse’s earlier (Rouse, 1996) proposals for a “post-modernist” philosophy of scientific practice could at least in part be cashed out in terms of (Deweyan) pragmatism. See also Pihlström, 2008.



Irreducible normativity, which is crucial for scientific practices to be rationally constrained, is to be found within paradigms themselves, not external to them.

White agreed with W.V. Quine already in the late 1940s and early 1950s that there is no sharp, essentialist dichotomy to be drawn between analytic and synthetic statements (see White, 1956). However, he extended this holism to cover the relation between factual and normative statements, which—in contrast to Quine—he also saw as entangled (White, 1986); ultimately, this leads to a comprehensive holistic philosophy of culture in which science as well as ethics, law, and history, among other fields of inquiry, are seen as constituting a single overarching “web” (White, 2002; cf. Pihlström, 2011b). This is a web of beliefs as much as a web of practices and activities of inquiry, going very well together with the classical pragmatists’ broad notion of inquiry, which covers not only science as conventionally understood but also ethics, politics, and even religion.

Moreover, such “webs” are historically developing entities, also in a way comparable to traditions, which clearly brings them close to Kuhnian paradigms. It is only within such a context—a paradigm, a web, a network—that something can count as a belief that could have a truth-value, as a way the world can be taken to be. So, we are here dealing with a transcendental issue again. The ways in which we are intentionally, experientially, and representationally connected with the world we inquire into through our webs of beliefs and practices are ultimately transcendental. They enable us to engage in our cognitive endeavors, both scientific and everyday ones. The world is never just “given” to us independently of such practice-laden, normatively constrained engagements. The webs of beliefs we may act upon are frameworks in terms of which the world can be scientifically represented.

The concept of *interdisciplinary inquiry* is particularly crucial here. Again, this is something that philosophers of chemistry might be able to appreciate better than some others: chemistry, after all, seems to be an inherently interdisciplinary field of science, deeply connected not only with physics but also with biology and applied sciences like medicine. I would like to add, therefore, some comments on how interdisciplinarity might be viewed in terms of holistic pragmatism.

One might even argue that White’s holistic pragmatism itself is not just a philosophical but also an inherently interdisciplinary approach to inquiry. The sciences and the humanities, in particular, are parts of the same holistic web of rational inquiry into the world we live in, just like science and ethics are. A holistic pragmatist conception of interdisciplinarity

should be able to integrate naturalism (or the legitimate emphasis on the natural sciences and their significant achievements) with something like humanistic “constructivism” (human self-interpretation and self-transformation) into a single, yet pragmatically pluralistic and open-ended, image of our rational inquiries into the nature of things, ourselves included. If, when engaging in such inquiries, one is literally surrounded by colleagues representing different disciplines, one may also be better equipped to understand one’s own inquiry as interdisciplinary; one may even cease to view oneself (or others) as a representative of a single discipline and rearticulate one’s own position in the field of inquiry as irreducibly interdisciplinary.<sup>6</sup>

I am *not* here pretending to know exactly what interdisciplinarity is, or how it should be defined. One key aspect of the pragmatist and fallibilist rejection of “first philosophy” (following Quine and White, as well as Kuhn and other practice-oriented philosophers of science) is, in any event, the acknowledgment of the need for deepening interdisciplinarity—not only multidisciplinarity—in our inquiries into the world and ourselves, including our inquiries into what scientific inquiries themselves are and should be like. One reason why holistic pragmatism is an inherently interdisciplinary approach in these inquiries (as I suggested above) is that pragmatists ought to oppose all dichotomies and boundaries that may “block the road of inquiry” (quoting Peirce’s famous words). Traditional disciplinary boundaries may be such blocks. They may, by blocking the road of inquiry, even block the emergence of certain kinds of scientific facts or objects that (only) an interdisciplinary paradigm makes possible.

Of course, in practice there may be cases in which it is difficult to determine what exactly interdisciplinarity should mean and how it ought to be promoted in practices of inquiry, or academic institutions. For example, in interdisciplinary research institutions, in practice at least three alternative “readings” of the requirement to promote interdisciplinarity, significantly varying in strength, might be implemented. (i) Each individual

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<sup>6</sup> It should be noted, however, that while these reflections are normative in the sense that I am to some extent recommending a more interdisciplinary approach in inquiry, a pragmatist philosopher of science should keep all doors open here: in many cases—in inquiries into a variety of important human problems—we should operate in terms of traditional disciplines rather than interdisciplinarily. This should be decided on a case-by-case basis depending on the specific needs and interests of the inquirers and their problems. Hacking’s (2002) concept of a “style of reasoning” would also be relevant here—possibly comparable to the notion of a “web” of inquiry invoked by holistic pragmatists—but I must leave detailed comparisons to another occasion.

scholar and/or research project might be required to be *internally* interdisciplinary (though possibly there can be degrees in the strength of their interdisciplinarity). Thus, no scholar or research project should, according to this formulation, represent just a single academic discipline but would have to represent at least two (or, perhaps preferably, more). (ii) According to a somewhat weaker interpretation, an individual scholar and/or project could represent just one discipline, but they would have to be open to interdisciplinary relations to other disciplines. There would thus have to be interdisciplinary *potential* in a research proposal, even though it would not have to be internally interdisciplinary. (iii) Only the interdisciplinary research institution as a whole would, according to the weakest interpretation, be required to be truly interdisciplinary. This would allow individual scholars and/or their projects to be even relatively strictly “disciplinary”, but their combination would be expected to be such that (perhaps unexpected) interdisciplinary cooperation might grow out of it. (I am not saying, of course, that these three options exhaust all the alternative formulations of interdisciplinarity.)

Now, how should the correct strength of the interdisciplinarity expectation (either in the case of an individual or in the case of a community of scholars) be determined? Does pragmatism, e.g., White’s holistic pragmatism or Kuhnian practice-oriented philosophy of science, help us in this regard? There is no immediate answer to the question of how strong interdisciplinarity pragmatism should promote. On the contrary, this is itself a contextually pragmatic matter, to be determined through a holistic critical consideration of the practices in question, in relation to other practices forming our cultural “web”, as well as the purposes of the inquiry we are engaging in. The pragmatic value of interdisciplinarity should, moreover, always be relativized to the aims and goals of the particular inquiry (or practice) thus contextually and holistically considered.<sup>7</sup> An obvious example of philosophical interdisciplinarity is the

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<sup>7</sup> See the previous footnote. As already emphasized, although I find interdisciplinarity an increasingly important challenge—and holistic pragmatism a philosophical framework that may be able to make sense of it in interesting ways—I by no means want to preclude traditional more “disciplinary” scientific research or diminish its importance. Traditional disciplines with their own methodologies (and even ontologies—in a practice- or paradigm-dependent sense) do have their role to play even in an increasingly interdisciplinary world of science. Their historically situated “styles of reasoning” (cf. again Hacking 2002) should never be simply abandoned for the sake of interdisciplinarity alone; our inquiries, whether disciplinary or interdisciplinary, ought to be driven by the problems themselves that arise from our human practices.

debate over *naturalism*—a debate to which pragmatists since Dewey have made major contributions and to which Rouse (2002) offers one of the most balanced reactions in the contemporary discussion—which cannot be settled independently of a vast variety of other philosophical and metaphilosophical issues, ethical and political ones included.

At this point of our discussion, it goes without saying that wide-ranging philosophical issues such as naturalism and interdisciplinarity are, in my view, also “transcendental” issues in the reinterpreted pragmatic sense explicated above. They are in the end issues concerning our being able to meaningfully represent reality. Furthermore, it has sometimes been suggested that, far from there being a sharp separation between the humanities and the natural sciences, all sciences are actually “human sciences”. Natural sciences like physics are themselves oriented to the world on the basis of human interests and needs. These are not “nature’s own” perspectives—recall again not just Kuhn but Kant and the classical pragmatists, too—but, inescapably, human ones. They are, as much as the traditional humanities, expressions of human self-interpretation. This is also something that pragmatists attracted by White’s holistic pragmatism could and should spell out in more philosophical detail, while including philosophy—as well as metaphilosophy—itself in the practice-embedded web of beliefs to be holistically tested. Science (including chemistry) is part of human culture, and when critically examining the normative structures of academic practices of inquiry, we already operate within holistic pragmatism, ultimately evaluating the “unified whole” of human culture more generally, i.e., our ways of being in the world and categorizing and inquiring into the world in and through the cultural practices we have developed and are continuously developing.<sup>8</sup>

#### 4. Scientific Realism?

At least one major philosophical question remains to be considered: *scientific realism*. As I have suggested above, pragmatism can, generally, be understood as synthesizing something like transcendental idealism (in its naturalized and historicized, thus contextually relativized, reincarnation) with empirical realism. This is a further indication of its deep commitment to a Kantian approach in the project of conceptualizing our cognitive and representational relations to reality. It should, thus, be easy to appreciate both the Kantian and the pragmatist aspects of not only Kuhn’s conception

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<sup>8</sup> This interpretation and elaboration of White’s holistic pragmatism is more comprehensively developed in Pihlström, 2011b.

of science but also, say, Putnam's internal realism (cf. Putnam, 1981, 1990).

In the realism debate, there are, of course, a wide variety of different views to consider—almost all of which must simply be ignored here. For instance, how exactly the pragmatist and Kantian elements of what I have called “pragmatic realism” (cf., e.g., Pihlström, 2008) might be incorporated in the slightly different position known as “practical realism” (Vihalemm, 2011) remains to be discussed elsewhere. I suppose that Rein Vihalemm's practical realism differs from my approach in being more distant from the Kantian transcendental concerns—and therefore in a sense “more realistic” (and at least not idealistic even in a reinterpreted sense). Yet, it seems to me that a very basic transcendental issue concerning the practice-laden representability and experience ability of reality must be taken up from the perspective of practical realism, too: according to Vihalemm's practical realist, scientific objects can, after all, only be identified within scientific practices. Thus, it would seem—at least this rearticulation should be available to the “Kantian pragmatist”—that practices provide transcendental (contextual) conditions for the possibility of there being scientifically representable objects at all—for us. This also sounds very much like Dewey's (e.g., 1929) view that scientific objects are not “ready-made” prior to inquiry but rather arise out of, or are constructed and/or identified in the course of, inquiry.

In addition, it must be observed that the problem framework of scientific realism raises issues not just concerning the traditional opposition between *realism* and *idealism* (today reconceived as the debate between *realism* and *constructivism*) but also concerning the ones between *realism* and *relativism* (compare the discussion of the “relativized a priori” above in section 3) and even *realism* and *nominalism*. I have commented on these issues, also in relation to the philosophy of science and its history—with the particular goal of understanding better the development of pragmatist philosophy of science in the twentieth century—on a number of earlier occasions (e.g., Pihlström, 2008, 2011c), so I will be very brief and selective here.

In the case of the realism vs. nominalism dispute, which might seem to be relatively far removed from the central issues in contemporary philosophy of science (it sounds more than slightly medieval, doesn't it?), the crucial question for a pragmatic realist and transcendental pragmatist is this: is there a viable analogy of (pragmatic) transcendental idealism and empirical realism when it comes to the special issue of realism about

*universals* (or what Peirce called “real generals”, e.g., laws and habits)<sup>9</sup> and/or *modalities*, both of which are crucially important in an adequate conception of scientific inquiry as an inquiry into something “real”? In previous works (Pihlström, 2003, 2009), I have offered a pragmatic-constructivist (albeit naturalized transcendental) account of Peircean “real generals”, acknowledging their reality but interpreting this reality only in a practice- and discourse-internal sense—that is, as something ultimately humanly “constructed” (cf. also, e.g., Margolis, 2010). The key idea here is that real generals, such as natural laws and dispositions, must be postulated in order to make sense of the scientific pursuit of truth, including truth about general laws and regularities, but this is nevertheless our human way of making sense of—or inquiring into what we find necessary conditions for the possibility of—*our* practices of inquiry.

Now, while something like this is certainly a philosophical view of real generals fitting “local” practice-oriented philosophy of science and science and technology studies—a realism about real generals that is analogous to “mere” empirical realism and therefore well compatible with transcendental idealism or constructivism (pragmatism)—we must still pause to reflect on whether the position we have arrived at is plausible or even coherent. Stronger Peircean realists may argue that pragmatism itself, given its method of focusing on the “conceivable practical effects” of our ideas, concepts, conceptions, and theories,<sup>10</sup> presupposes in a more full-blown sense the basic commitments of what Peirce called “extreme scholastic realism”, i.e., realism about generality, including modalities. This is, arguably, because a realistic interpretation of possibility, in particular, is needed in order to account for “conceivable practical effects”. The conceivable effects our ideas may have include effects never concretely realized in actuality.

This sounds heavily metaphysical but is in fact a vital issue for pragmatist philosophy of science, too, not just for pragmatist metaphysics. Are, for instance, physical or chemical laws and other structures Peircean-like “real generals”? If so, is it plausible to claim that they are still somehow transcendently dependent on our inquiry, in a (pragmatically

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<sup>9</sup> For more details, see Peirce’s early and late writings on “real generals”—all the way from the late 1860s to 1905–1907—collected in Peirce, 1992–98. For references to relevant scholarship, see also Pihlström, 2009, chapter 6.

<sup>10</sup> This is not the proper place to inquire into the meaning of the pragmatic method or pragmatic maxim, first formulated by Peirce in his 1878 essay, “How to Make Our Ideas Clear” (reprinted in Peirce, 1992–98, vol. 1), and later employed by James, among others (see especially James, 1907, chapter 2). For an updated discussion, see the relevant contributions to Pihlström, 2011a.

reinterpreted) Kantian-like sense? Are natural laws, in particular, nomically necessary in a realistic sense; are they also “real generals”? And even if they are, aren’t they also metaphysically (as well as, of course, logically) contingent, as the law-like structure of the world could presumably have been very different from what it *de facto* is? What is, furthermore, the relation between scientific representations (contextualized in our inquiries) and the laws that are from the point of view of our scientific theories claimed to “really” obtain in the world?

These issues remain open here; in any event, my general proposal is that real generals can and should be regarded *not* as features of the world *an sich*—any more than our theories or representations can ever be about things in themselves, either according to Kant or according to Kuhn—but as features of the-world-as-seen-through-the-practices-of-inquiry (whatever that ultimately concretely means). For example, chemical structures could be seen as both real (that is, as real generals independent of our representations in an empirical sense) and as constructed (that is, as practice- or paradigm-relative, or at least identifiable only within practices or paradigms, in the pragmatically naturalized transcendental sense). More work clearly needs to be done here.

One way of pragmatically “cashing out” the idea that what there is depends on our epistemic and representational activities and practices of inquiry—or, in Kuhnian terms, on our paradigms—and the related idea of integrating transcendental idealism (constructivism) with empirical realism, through pragmatism, is what I have elsewhere called the “contextualization of scheme-(in)dependence” (see Pihlström, 2011c). The basic idea here is that *nothing* is scheme- or practice- (or paradigm-) dependent or -independent *as such*, “in itself”, but only in one or another context of practice-driven inquiry. Hence, the contextuality and relativity of a priori principles (cf. section 3 above) is in a way taken to the meta-level of philosophical interpretations of transcendental philosophy and the notions of scheme- or practice-dependence and scheme-independence themselves.

Even so, the question concerning realism about generality, particularly about real possibilities and other modalities, must be left unresolved here. Philosophers of science often find it necessary to invoke irreducibly modal notions in order to make sense of the idea that the world *could* be, or could have been, structured in terms of quite different practice-embedded theories and paradigms than the ones we actually have at our disposal.<sup>11</sup>

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<sup>11</sup> For example, Rom Harré’s suggestion that the world, “prior to” conceptualization and measurement (or the application of an apparatus of investigation), is somehow a world of “affordances”, potentialities, or powers,



Somehow modalities must already be incorporated in practices themselves, so it is not enough to simply say that a (moderately) realistic interpretation of modalities is just based on our practices. After all, practices are contexts within which things can be done in certain ways—or occasionally left undone—and this clearly means that they are, in Peircean terms, “generals”. So are Kuhn’s paradigms. So are any contexts that can play the transcendental role of pragmatically enabling scientific representation of objects, in the sense outlined in the early sections of this paper.

## Conclusion

The relevance of all this relatively abstract and general discussion to both the interdisciplinary field of science and technology studies (or other practice-oriented reflections on the nature of science) and to special fields within the philosophy of science, such as the philosophy of chemistry in particular, must remain implicit. However, the general issue of realism and the questions concerning the pragmatic naturalizability of transcendental approaches to that issue could presumably easily be illustrated in terms of more specific problems drawn from current discussions in these fields.

Pragmatism, I have tried to argue in this paper (and in some more detail, albeit in somewhat different contexts, in several previous publications), is a highly promising philosophical (and metaphysical) perspective in these inquiries, but it needs both updating in terms of interdisciplinary, “localized” investigations of scientific practices (e.g., from the perspective of science and technology studies as a “successor” of traditional philosophy of science) and Kantian backing, or what might be called “retranscendentalization”. We must not forget that, even when dealing with “local” issues of the identifiability of objects within practices and the roles that our practices and/or paradigms (may) play in the constitution of reality as knowable and representable by us we are dealing with transcendental topics. Philosophy of science does not, and must not, give up those fundamental traditional concerns simply by turning pragmatic and non-foundationalist; through that turn it merely reinterprets

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comes close to a view admitting Peircean real generals. However, Harré emphasizes that these potentialities are not exactly “in” the world itself prior to its being subjected to an investigation involving our apparatuses; they are properties of “the world plus the apparatus”. This makes his view clearly pragmatic (yet, in my view, also transcendental). (I am indebted to discussions with Rom Harré in the workshop on practical realism in the philosophy of science at the University of Tartu, June 2011, regarding these issues.)



them in novel ways. The same holds for special fields within philosophy of science, such as the philosophy of chemistry in particular.<sup>12</sup>

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# **ANALYTICAL APPROACHES**

# THREE METAPHYSICAL ISSUES IN CHEMISTRY

ROBIN FINDLAY HENDRY

## Introduction

A primary task for the philosophy of chemistry is to provide an account of what the world is like, according to modern chemistry, in the respects in which chemistry studies it. This involves studying its currently accepted theories and the implicit assumptions underlying its practices, and thinking about how the world would be, in the respects in which chemistry studies it, if those theories and assumptions were broadly true. One might call this project an immanent metaphysics of chemistry. It is immanent in the sense that its picture of chemical reality is guided (so far as possible) by claims from within chemistry itself, rather than by any self-appointed transcendental perspective that seeks to place limits, from outside chemistry, on the scope of its claims, or on their epistemic status. It is metaphysical in two ways. Firstly, it concentrates on how chemical reality *is* (represented to be) rather than how chemists know about it. Secondly, it is helpful to draw on various theories and arguments from metaphysics, in the hope that they may help us fill out chemical theories more fully, or help us decide between possible interpretations. It may not always be relevant to chemists to fill out an ontological picture in detail, or to decide between two or more possibilities. Bringing in metaphysics might seem to undermine the *immanence* of this approach, but it need not: Metaphysics provides various theories of how things might be, developed in more detail than other areas of inquiry. In fact the development of such theories is its core business. But these insights need not be *imposed* on chemical theory: Rather they are resources to be put at its disposal.

We stand to learn something from this project because chemistry has, for the past two hundred years, made a major contribution to knowledge by successfully gathering evidence and constructing theories about the nature and structure of chemical substances. Moreover, the philosophical debate about scientific realism encourages us to worry about *retention*: How far the successful theoretical claims of earlier scientific epochs are preserved in later science. This is a real worry in physics, where Newtonian mechanics has given way to classical and then relativistic dynamics, but

chemistry's current body of theory appears to have been gathered in a more cumulative fashion. In the late eighteenth century, Lavoisier showed that oxygen and hydrogen are components of water. Modern chemistry still deems them to be so, adding claims about the proportions of that composition in the nineteenth century, then a formula to represent that proportionality, and finally a structural interpretation of that formula. So we might reasonably expect to learn something about the nature of substances by carefully and critically examining its theories. Whatever the ultimate fate of chemistry's current theoretical claims, they are not passing fashions.

Immanent metaphysics is not the only way to look at chemistry. From time to time philosophers, historians and sociologists set out other perspectives with which to approach the theory and practice of science in general, or of one particular science. Each such perspective has its own motivations, its own rules of interpretation, and consequently its own merits and demerits. For instance, a perspective might be inspired by the philosophical tradition of empiricism, or of classificatory nominalism, or the anthropological tradition of suspending the commitments of one's own culture. We may well learn much from these perspectives, though we should be careful not to confuse the fundamental posits of an approach with the results of its interpretation. If empiricism, classificatory nominalism and the symmetry principle are imposed from the start then they are not something we find in the raw data. Moreover we need to be aware of the particularity and contingency of these perspectives: It shouldn't be assumed that their fundamental posits are inevitable, transcendental requirements which can then be used as a basis on which to interpret chemistry. They may only generate pseudoproblems for chemistry in terms that are unrecognisable from the point of view of that science.

## **1. What is a Chemical Substance?**

Modern chemistry names chemical substances for their microstructures. That can quickly be established by considering the International Union of Pure and Applied Chemistry's rules for nomenclature and classification (see for instance Thurlow 1998). Microstructure is also the basis of chemical explanation. The chemical and physical behaviour of a substance can be predicted and explained at least qualitatively (and defeasibly, of course) by reference to its microstructural properties. For instance there is no explanation of spectroscopic behaviour except that which flows from how, given its molecular structure, a substance interacts with radiation of

various frequencies. So, chemistry individuates substances via their microstructural properties, in the sense that microstructural properties determine the extensions of the names of substances. In other papers I have defended this claim, known as microstructuralism (see Hendry 2006, 2008a), but here I would like to concentrate on its consequences, and in particular its consequences for what chemical substances are. I will not here consider the alternative macroscopic conceptions of substances (see Needham 2000, 2002, 2008, 2011; van Brakel 2000 Chapter 3, 2012). Although interesting and significant, I think that these conceptions of substance are motivated by concerns that, since the beginning of the twentieth century, have been foreign to the discipline of chemistry (see Hendry 2006, 2010a, 2010e).

Before I continue I should address a question about this whole project: Surely no metaphysical conclusions of any kind follow from the mere fact that chemists adopt one particular set of linguistic conventions rather than any other? The question can be rejected because it rests on a false assumption. The IUPAC rules are not linguistic conventions, because they embody substantive hypotheses about the microstructure of chemical substances, and which aspects are important for understanding their behaviour. Here's another way to see the role of nomenclature: Joseph Priestley complained that the New Nomenclature introduced by Lavoisier and others embodied substantive assumptions about the composition of chemical substances. He was right about the theoretical commitment of the New Nomenclature, but wrong to identify it as illegitimate.\* In the Preface to the *Traité Élémentaire de Chimie* (Lavoisier 1790), Lavoisier was quite explicit in his argument for nomenclature reform that the new names for substances should reflect their composition. Nowhere does he say that chemical names should be free of theoretical commitment (perhaps they should be free of *unjustified* theoretical commitment, but that's a different thing). The survival of the binomial nomenclature, and the great success of (part of) Lavoisier's scheme in contributing to the scientific understanding of composition and combustion are evidence for the truth of the assumptions underlying that scheme.

The structural nomenclature of the modern IUPAC rules embodies a view of molecular reality according to which similarities and differences

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\* Priestley was right of course to worry that, in excluding phlogiston, the new nomenclature precluded it from having a compositional, and therefore an explanatory role. But that is a worry about error: the error in neglecting phlogiston's role in combustion. It reflects the viewpoint of someone who is committed to that role. The worry need not be shared by anyone who does not share the commitment.

in the chemical and physical behaviour of substances are determined by similarities and differences in their molecular structure. The close connection between nomenclature, classification and theoretical explanation is beautifully illustrated in organic chemistry, where explanations proceed precisely by fitting a particular substance into a classificatory framework based on structure, and then understanding its properties and behaviour in terms of its similarities and differences from near neighbours. Moreover, the predictive and explanatory use of this framework has been highly successful. As G.N. Lewis put it:

No generalization of science, even if we include those capable of exact mathematical statement, has ever achieved a greater success in assembling in simple form a multitude of heterogeneous observations than this group of ideas which we call structural theory. (Lewis 1923, 20-1)

Surely these ideas deserve to be taken seriously if any body of scientific hypotheses does. And taking them seriously means taking seriously the idea that, at every level, structure and composition are what make a substance what it is, and determine how it behaves.

With these preliminaries, we can begin to draw some metaphysical conclusions. Firstly, if chemical substances are individuated by their microstructural properties, then there can be no distinction between chemical substances without accompanying distinctions in their microstructural properties. So the identity of chemical substances supervenes on microstructure. Secondly, if chemical substances are the substances they are in virtue of their microstructural properties, then they (substances) cannot exist unless the bearers of microstructural properties—that is, molecules and other such microscopic species—exist. As a consequence, chemical substances depend ontologically on their constituent microspecies. Now add a further plausible principle: Not only are chemical substances characterised and individuated by their microstructural constituents, they are exhausted by them. Chemical substances have no components that are not microstructural species. An elegant way of unifying and explaining all these facts is the hypothesis that chemical substances are *modes*: Ways for collections of molecular species to be.

However, microstructuralism has in the past been rejected for its commitment to false (or at least unjustified) claims: That chemical substances are homogeneous at the molecular level, that atoms are indivisible, and that the chemical is reducible to the physical. In fact microstructuralism need bear none of these commitments.

Pierre Duhem once argued that



Dalton's thought remains perfectly clear. Simple substances are formed of *atoms*. The atoms of the same simple substance are all alike; they have the same mass. ... All compound substances are reducible to *molecules*. The molecules of a given compound are all identical with one another; each is formed from a certain number, necessarily whole, of atoms of each simple substance which combine to bring about the formation of the compound (2002, 86).

Likewise Jean Timmermans (1941, Chapter VIII) presented the "particle or corpuscular theory" of substances as defining elements as classes of "*identical molecules* containing a *single species* of *atoms*: O<sub>2</sub>, S<sub>8</sub>, P<sub>4</sub>, Hg, etc.", while compound substances consist of "*identical molecules* each containing *several species* of *atoms*: NaCl, CH<sub>4</sub>O etc." (1941, 45). Timmermans presented isotopy as an objection to the atomist view of elements. Now Dalton and Mendeleev were indeed committed to the idea that the atoms of a particular element are qualitatively identical to each other, but this idea played no role in the explanatory power of the atomic theory in accounting for the laws of definite and multiple proportions. The theory did assume that atoms are alike in their mass, but similarity in any other respect was unnecessary. Timmermans is quite right that isotopy showed that even the weaker thesis was false, but a more charitable view of the atomism of Dalton and Mendeleev would consider also the weakest version of their theory that could explain the laws of definite and multiple proportions: This would be the assumption that atoms share some important property. On this charitable view, although there was some truth in the atomist explanation, Dalton and Mendeleev misidentified the atomic property shared by the atoms of an element. Moreover they misidentified it for good reasons: Atomic weight was the only atomic property that they had (imperfect) epistemic access to; and atomic weight is correlated with nuclear charge, the property that actually determines the chemical behaviour of an atom.

It is similarly unclear why nineteenth-century chemical atomism was so firmly associated with the assumption that atoms are indivisible, since the connection with ancient atomism is distant. Elements must survive *chemical* change in order to play their allotted explanatory role, but that would allow that they may be altered in other respects. William Whewell (1847 Volume I, 422-3) pointed out the explanatory idleness of the assumption of the indivisibility of atoms, but like Timmermans he saw this as a criticism of atomism, rather than the occasion for charitable reinterpretation. In this context Timmerman's isotopy criticism is also odd because the property that the atoms of an element were discovered to share was *another* atomic property, namely nuclear charge. In any case, isotopy

has no tendency to undermine microstructuralism, which views elements as populations of atoms of like nuclear charge, which may be heterogeneous in other respects (see Hendry 2006, 2010a for articulation and defense).

Among proponents of microstructuralism, Putnam once suggested that the extension of “water” should be identified with “the set of all wholes consisting of  $\text{H}_2\text{O}$  molecules” (1975, 224), which I take to mean that a body of water should be thought of as a mereological sum of  $\text{H}_2\text{O}$  molecules. Now I have no doubt that the term “water” is sometimes used to refer to mereological sums of water molecules, but ordinary water is not, of course a mereological sum of any uniform class of molecules. Rather, it contains a disuniform array of different microscopic species, including hydrogen-bonded networks of  $\text{H}_2\text{O}$  molecules, protons, and hydroxyl ions. But this fact has no tendency to undermine microstructuralism, which need not require that substances are homogeneous populations of molecular species, or even that every member shares some property (though elements are homogeneous in that way). The requirement is only that the populations as a whole have some significant microstructural property. To make the theory informative, one must identify that property of course. To that end I have argued that water is the substance that forms naturally when  $\text{H}_2\text{O}$  molecules are brought together and interact to produce the disuniform molecular populations that actually characterise liquid water (see Hendry 2006, 2008a). In conclusion, the microstructuralist proposal is disjunctive: Chemical substances are either natural classes of molecular species (that is, molecules which share some significant structural property), or molecular populations produced by natural classes of molecular species when these species interact with each other.

## 2. What is Structure?

The thought that structure is central to chemical classification and explanation raises the question of just what, in general, structure *is*. In the most abstract terms, the structure of a thing is just the way its various parts fit together to make up the whole. That is too abstract to be informative on its own: To say something more definite we need to identify what the parts are, and which aspects of the way they fit together are important to chemistry. In keeping with the immanent approach of this paper, we can extract this information from chemistry’s own representations of structure, and from chemists’ interpretations of these representations. It is perhaps unsurprising that different branches of chemistry have given rise to

different representations of structure that correspond, presumably, to the different kinds of structure which are important in understanding the chemical and physical behaviour of the kinds of substances they study. An important distinction comes between the ionic crystals characteristic of salts and the molecular substances characteristic of organic chemistry. On the one hand ionic crystals like sodium chloride can be understood, to a first approximation, as being assembled from ions of opposite signs arranged into repeating series of unit cells. The stability of the structure arises (again, to a first approximation) from electrostatic interactions between opposite charges. On the other hand the structure of discrete molecular substances is represented in the molecular structure diagrams (or valence formulae) which have been central to explanation in organic chemistry since the 1860s: Here the structure arises from bonds between individual atoms.

There are important differences between the two kinds of structure. The first difference concerns the source of the structure. As G.N. Lewis pointed out (1913, 1452), the bonding in an ionic solid involves no linkages between particular pairs of ions, because any ion interacts equally with each of its oppositely charged neighbours. In contrast the structure diagrams of organic chemistry are precisely *relational* structures because they are generated by individual relationships between atoms. In fact they were recognised as describable within graph theory as early as the 1860s (see Biggs et al. 1976, Chapter 4). The second difference concerns the dynamical behaviour of these structures. The repeating cell structure of an ionic solid can be characterised as involving (average) spatial relationships between the constituent ions, and the structure cannot survive large deviations from these relationships. In contrast, the structure of a molecule is compatible with many different spatial relationships between its constituent atoms. Of course a bond between two atoms does constrain the distance between them, but the distance between two non-neighbouring atoms in a structure may vary widely as different parts of the molecule move relative to each other under the constraint of their bonds (think of the conformations of cyclic alkanes). If molecular structures are not just specifications of spatial relationships between atoms then perhaps they ought to be understood *functionally*, as relational structures generated by the bonding relation, although since van't Hoff they have been relational structures embedded in three-dimensional space. The bonding relation is itself to be understood as a creature of the structural explanations of nineteenth-century organic chemistry.

Now if the explanatory role of the chemical bond began to be mapped out in the nineteenth century, the task of identifying what realises that role

fell to twentieth-century chemists and physicists. Lewis (1923) provided the first widely accepted account: The electron-pair bond, which unified chemists' understanding of bonding in polar substances (like sodium chloride) and non-polar substances (like methane). The electron-pair bond also helped to create a whole new level of understanding of reaction mechanisms in organic chemistry during the 1920s and 1930s (see Goodwin 2007), and continues to be central to understanding reaction mechanisms in that subdiscipline (see Goodwin 2012). Lewis' ideas also played an important part in early quantum chemistry: Applying the first principles of quantum mechanics to molecules turned out to be far beyond 1930s computational abilities, so semi-empirical bonding models were developed, such as the valence-bond approach championed by Linus Pauling, who regarded it as a synthesis of quantum mechanics with Lewis' ideas (Hendry 2008b). Although Pauling's efforts provided quantum mechanics with some important early successes, such as an explanation of the tetrahedral structure of bonds around the carbon atom, the valence-bond approach was just one approximate scheme among others (the chief rival being molecular-orbital theory), and the chemical structure seemed to have been put into the quantum mechanics by hand rather than derived *from* it. Moreover, Lewis' localised pairs of electrons seem quaint from the point of view of subsequent theory. There were well-known physical arguments that molecules must be dynamic entities, constantly in motion, and that the electrons within them could not therefore be static (see Sutcliffe and Woolley 2012). Quantum mechanics only makes things worse, in two ways: Firstly, electrons are delocalised within molecules; secondly they are fermions, which means that the electronic states of molecules must be anti-symmetric with respect to electron permutation. Hence if they are to be realised by molecular quantum states, individual bonds cannot be understood simply as individual pairs of electrons. For all these reasons, some physicists and theoretical chemists have been sceptical about whether bonds can be regarded as a genuine feature of quantum-mechanical reality, even though they seem indispensable to chemical explanation (see Hendry 2004, 2008b). Bonding is, of course, a real phenomenon: The question is whether understanding this phenomenon requires something like the *structural* chemical bond of the nineteenth century, and how far quantum mechanics is compatible with it (see Hendry 2008b; Weisberg 2008). Should the structural conception of the bond be discarded in favour of something that is unproblematic at the level of the underlying physics? A more physically respectable conception of the bond might just identify it with the energetic stabilisation of a molecular system. It is doubtful, however, whether this conception of the

bond is rich enough to capture the explanatory role of the bond in organic chemistry. A more direct objection to this energetic view arises from the exotic chemical species discussed by Jerome Berson (2008). Berson argues that extending quantum-mechanical analysis to the “fleeting molecules and molecular fragments” (2008, 956) that appear in the course of chemical reactions, challenges some long held assumptions about chemical bonds. One such assumption is that the formation of a bond must always stabilise a molecule: Berson provides examples in which a non-Kekulé species may be of lower energy than its Kekulé isomer, because the structural constraint exerted by the additional bond may distort other parts of the molecule into higher-energy configurations (2008, 952). Without the bond, the molecule can relax into a less strained shape.

An alternative to the austerity of the energetic conception is to pick up on the idea, floated earlier, that the notion of a chemical bond should be identified with its role in structural explanation. The issue is then to identify the physical realiser of this explanatory role. In the “Atoms in Molecules” programme, Richard Bader and his co-workers have sought to recover the traditional bond structure of molecules as a topological feature of the electron-density distribution (see Bader 1990; Gillespie & Popelier 2001). From the electron-density distributions for many different molecules can be defined “bond paths” between atoms that generate “molecular graphs” which are strikingly close to the classical molecular structures of those molecules. As Bader puts it, “The recovery of a chemical structure in terms of a property of the system’s charge density is a most remarkable and important result” (1990, 33). The philosophical interest of Bader’s elegant results is twofold. Firstly, if the scheme were extensionally adequate, finding bonds just where classical valence formulae would put them, this would suggest that it provides some real insight into the underlying physical realisation of the chemical bond. If bonds are anything, they are topological features of a molecule’s electron-density distribution. Secondly, the fact that this account is based on electron density, which is undeniably a quantity of fundamental significance in quantum mechanics, suggests that the classical structural conception of the bond can be regarded as quantum-mechanically rigorous after all. But the correspondence between bond path and chemical bond is not perfect. The main problems concern *repulsive* (rather than attractive) interactions between neighbouring atoms in a molecule. Troublesome cases are provided by phenanthrene, and the inclusion complex of helium in adamantane (see Haaland et al. 2004 and Poater et al. 2006). Atoms in Molecules finds bond paths corresponding to these repulsive interactions even though chemists would not normally regard the mutual repulsions as

bonds. One response (see Bader 2006) is to point out that Atoms in Molecules embodies a *revisionary* conception of structure, and may find “bonds” where chemistry has traditionally put them. This is a reasonable response, but too much revisionism will tend to undermine the claim that molecular structure really has been recovered, and therefore the argument that the physical realiser of the bond has been successfully identified.

### 3. How does all this Relate to the Question of Reduction?

We now come to the third metaphysical issue. The thought that the entities and processes studied by chemistry just *are* physical, and that their behaviour can be exhaustively understood in terms of physical laws, is motivated by the close explanatory interaction between chemistry and physics. But it is not the only independently plausible view that is consistent with the evidence. Now in fact there are two layers to the question of reduction in chemistry. The first layer concerns whether chemical substances are nothing over and above their constituent microspecies. The next layer concerns the relationship between molecular structure and physics: Are molecules just quantum-mechanical systems of charged particles? I will address the first question only to note that microstructuralism about chemical substances does not commit one to reductionism about them: Even if substances are individuated by their microstructural properties, this does not entail that they are nothing over and above the bearers of these properties (for argument see Hendry 2008a, 118-9). The second reduction issue merits a longer discussion.

Quantum chemistry is the interdisciplinary field that applies quantum mechanics to atoms and molecules in order to explain their structure, bonding and reactivity. Textbooks often present the application as follows: We enumerate the electrons and atomic nuclei present in a molecule and identify the forces acting between them. This determines a Schrödinger equation for the molecule, whose solutions correspond to the quantum states it may have. Schrödinger equations for chemical systems typically consider electrostatic interactions only, which is a reasonable approximation because the other interactions (gravitational, weak and strong nuclear forces) are orders of magnitude weaker at the molecular scale, and can effectively be ignored where chemical behaviour is concerned. There is an exact analytical solution to the non-relativistic Schrödinger equation for the hydrogen atom and other one-electron systems, but these cases are special owing to their simplicity and symmetry properties. The Schrödinger equation for the next simplest atom, helium, cannot be solved analytically, and to solve the Schrödinger equations for more complex atoms, or for any

molecule, chemists apply a battery of approximate methods and models which have become very sophisticated with the development of powerful computers.

However, interesting issues of principle are raised not by atomic but by molecular structure. Can we regard this general phenomenon as being *explained* by Schrödinger equations as applied to systems of charged masses interacting electrostatically? Arguments that bear on these issues have been presented by Brian Sutcliffe and R.G. Woolley (see for instance Sutcliffe and Woolley 2012). One problem concerns isomerism. Ethanol ( $\text{CH}_3\text{CH}_2\text{OH}$ ) and dimethyl ether ( $\text{CH}_3\text{OCH}_3$ ) are different compounds with distinct molecular structures, but contain precisely the same electrons and nuclei. If a Schrödinger equation is determined only by the electrons and nuclei present then the alcohol and the ether share a Schrödinger equation, and it is difficult to see how their structures could be recovered from it (see Woolley 1998). Symmetry properties pose a deeper problem: Arbitrary solutions to exact Coulombic Schrödinger equations should be spherically symmetrical, but real molecules cannot be (see Woolley and Sutcliffe 1977, 2005). The problem is usually avoided by disregarding the exact Schrödinger equations in favour of lower-symmetry structures. This is motivated by the Born-Oppenheimer (or “clamped nucleus”) approximation, which separates the nuclear and electronic motions, then considers the massive slow-moving nuclei to be approximately at rest. Only the electrons are assumed to move quantum-mechanically, and while this makes little difference to the energy of the solution, it would seem fair to say that the internuclear structure is effectively assumed rather than explained. It is worth emphasising that this symmetry problem has nothing to do with the insolubility of Schrödinger equations for molecules, or the computational complexity of numerical methods for solving them. According to Woolley and Sutcliffe, the problem is not that molecular structure is difficult to recover from the Coulombic Schrödinger equations for isolated molecules, but that it is not there at all.

One reductionist response is that approximations are common in computationally complex parts of physics, and do not signal any deep explanatory failure. There is something in this response, but it requires that atomic and molecular models that are used in explanations are justifiable as approximations to solutions of exact Schrödinger equations, and stand in for them in explanations of molecular properties (hence, call this the “proxy defence” of inexact models). This is a more stringent condition than it may sound, requiring that the inexact models attribute no explanatorily relevant features to atoms or molecules that cannot be justified in the exact treatments. The Born-Oppenheimer approximation



seems to offer a justification for the assumed semi-classical molecular structures, because the masses of atomic nuclei are thousands of times greater than those of electrons, and so move much more slowly. Fixing the positions of the nuclei makes little difference to the calculated energy, so in calculating the electronic motions the nuclei may be considered to be approximately at rest. But if Woolley and Sutcliffe's symmetry argument is correct, the proxy defence would seem not to apply, because the symmetry properties of the Born-Oppenheimer models are explanatorily relevant, yet they cannot be justified in the exact treatments.

It is clear that the clamping of nuclei cannot really be regarded as an approximation, because although it makes only a small difference to the calculated energy of a molecule, it makes a big difference to its symmetry properties. To give an example, chirality is a form of molecular asymmetry in which a molecule is not superimposable on its mirror image, for instance because a carbon atom is bonded to four different groups of atoms. Hence chirality gives rise to a form of isomerism, and it has been known since the nineteenth century that in some cases the two isomers will rotate plane-polarized light in opposite directions, but by the same angle. If a determinate molecular structure is *assumed* (as, for instance, within the Born-Oppenheimer approximation), then it is possible to calculate the observed optical rotation angles. Exact solutions to the isolated molecule Hamiltonian, in contrast, will yield an optical rotation angle of zero. The symmetry problem is not specific to optical activity: Asymmetries in molecular structures are essential to all kinds of explanation at the molecular level.

One obvious response to these arguments is that of course structure cannot be recovered just from the Schrödinger equation for an isolated molecule. It should not, perhaps, be surprising if a Hamiltonian that was set up to describe an isolated molecule fails to apply in the bulk-matter environments that are of interest to chemistry. A determinate molecular structure must therefore be something a quantum-mechanical system of nuclei and electrons could, in principle, have or lack, depending on its interactions with its environment. Those who are comfortable with the idea of physics revising or even eliminating the central explanatory concepts of the special sciences might instead say "so much the worse for molecular structure." Although physicists of the stature of Max Born have said similar things (see Hendry 2004), there is a vast amount of chemical and spectroscopic evidence that chemists currently explain by appeal to determinate molecular structures. It is easy to advocate radical revision of existing explanations, but a lot harder to come up with the required revisions. Until there are new explanations of (for instance) carbon



dioxide's chemical and spectroscopic behaviour, or the complex mechanisms of organic reactions, explanations that do not appeal to determinate molecular structure, the call for explanatory revision is idle. A subtler version of this eliminativist view is to regard molecular structures as artefactual even while recognising their utility (or even indispensability) to chemical explanation. For instance, according to Hans Primas (1975, 1983), quantum-mechanical holism means that it is an idealisation to suppose that a molecule has a quantum state to call its own, a state that then interacts with its environment. All there is, from a quantum-mechanical point of view, is the state of the system-plus-environment (in effect, the universe as a whole). The quantum-mechanical properties normally associated with structure (determinate internuclear distances, moments of inertia) are not derived from an exact quantum-mechanical description. Rather, explanation in quantum chemistry involves the construction of model states that replicate the phenomenal patterns we read into a structureless quantum world (see Hendry 1998, 127-30 for a more detailed account of Primas' views).

Now the reduction issue does not begin and end with the relationships between theories we have been discussing here. Intertheoretic reduction of  $X$  to  $Y$  concerns whether or not a theory about  $Y$  entails the currently accepted theory about  $X$ , or entails an approximate version of it, or perhaps explains everything that that theory explains. Ontological reduction concerns whether or not  $X$  *itself* is something "over and above"  $Y$  in some robustly metaphysical sense that may be independent of any logical, mathematical or explanatory relationships between current or future theories about  $X$  and  $Y$ . In recent philosophy of mind, ontological reducibility has been understood in terms of causal powers:  $X$  is ontologically reducible to  $Y$  only in the case that the causal powers conferred by possession of  $X$ -properties are exhausted by those conferred by possession of  $Y$ -properties (see Kim 1998, chapter 4). On this formulation, neither ontological dependence nor microstructural supervenience (as established between substance and microstructure, above) is sufficient for ontological reduction, for the  $A$ -properties may confer "additional" causal powers. If, for each cluster of  $Y$ -properties corresponding to an  $X$ -property, there is a *sui generis* law of nature conferring distinct causal powers that are not conferred by more fundamental laws governing the  $Y$ -properties, then the  $X$ -properties are irreducible to the  $Y$ -properties in a robustly ontological sense. Is this more than a mere logical possibility? Woolley and Sutcliffe's symmetry problem would seem to indicate that it is. For over a century, chemical explanations of the causal powers of molecules, and of the substances they

compose, have appealed to molecular structures attributed on the basis of chemical and physical evidence. Yet the existence of such structures does not appear to have an explanation in the exact quantum mechanics of isolated systems of electrons and nuclei. If the explanation of molecular structure is that it arises from a quantum-mechanical system's interactions with its environment, then the truth or falsity of the reductionist view of chemistry will depend on the precise nature of this explanation. To be an ontological reductionist is to think that molecular structures arise from more fundamental laws, so the reductionist must expect that the ability of the environment to collapse the molecular symmetry is ultimately due to its falling under some more fundamental physical law. The opposing emergentist view is that for each molecular structure there is a *sui generis* law of nature that can be expressed in the language of quantum mechanics, but is an instance of no deeper physical law. To address the issue of the ontological reduction of chemistry is to assess the relative plausibility of these two interpretations, and how well they account for the explanatory relationship between physics and chemistry. The issue is not settled by the existence of quantum-mechanical explanations of molecular structure and bonding. Both reductionism and emergentism are compatible with there being such explanations, although they differ over their structure, and the degree to which the laws that appear in them are unified. It seems that the issue of reduction in chemistry is more open than philosophers have assumed (see McLaughlin 1992 and Hendry 2010b, 2010c, and forthcoming for differing views).

## Conclusion

Although structure and the chemical bond have received relatively little attention from philosophers so far, they are promising topics in the philosophy of chemistry, especially if we wish our subject develop in dialogue with chemists. The first topic I addressed in this paper (the nature of chemical substances) is not one with which modern chemistry actively engages: Chemical nomenclature, and the implicit assumption that chemical explanation should appeal to structure and composition, have dead science since the early twentieth century. My final topic, reduction, is generated primarily by general philosophical considerations. We philosophers have no reason to expect chemists to find either topic interesting. In contrast, the chemical bond is a notion with which every chemist is familiar, and is central to chemical explanation. Yet every theoretical chemist knows it to be a foundational puzzle, and as we have seen, its physical basis continues to be a topic for debate. Here

philosophers might hope to clarify the arguments and make more explicit the opposed positions and their disagreements.

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# MEREOLOGICAL STRUCTURE IN CHEMICAL SUBSTANCES AND THEIR TRANSFORMATIONS: AN ANALYTIC PERSPECTIVE ON THE HISTORICAL DEVELOPMENT OF THESE CONCEPTS

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## Introduction

The term “mereology”, deriving from the Greek word *meros*, part, was coined by Lesniewski in 1914 for the algebraic system of relations and operations built up from the dyadic “part” relation.<sup>1</sup> The application of mereology in geometry was introduced by Huntington (in substance if not by name) and Tarski.<sup>2</sup> Leonard and Goodman introduced it into analytic philosophy,<sup>3</sup> and it continues to be much discussed in contemporary analytic metaphysics. Here I will discuss the application of mereology in the understanding of concepts from chemistry.

Much of my work in the philosophy of chemistry over the past decade or so has been concerned with the development of the concept of chemical substance along with allied concepts such as phase and process. This has

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<sup>1</sup> The term “merology”, without the second “e”, was already in use for the now obsolete part of anatomy concerned with elementary tissues and fluids. Peter Simons, “Real Wholes, Real Parts: Mereology Without Algebra”, *Journal of Philosophy*, 103 (2006), 597-613; p. 599, fn. 5, conjectures that this is why in 1914 Lesniewski coined the irregularly formed term “mereology”.

<sup>2</sup> Edward V. Huntington, “A Set of Postulates for Abstract Geometry, Expressed in Terms of the Simple Relation of Inclusion”, *Mathematische Annalen*, 73 (1913), 522-559; Alfred Tarski, “Foundations of the Geometry of Solids”, trans. of original 1926 article in *Logic, Semantics and Metamathematics*, Hackett Publishing Company, Indianapolis, 1983.

<sup>3</sup> H. Leonard and Nelson Goodman, “The Calculus of Individuals and Its Uses”, *Journal of Symbolic Logic*, 5 (1940), 45-55.

led me to the view that up to around the beginning of the twentieth century, these concepts were essentially what would now be called macroscopic concepts. The development of a coherent theoretical basis for the understanding of the microstructure of matter from the beginning of the twentieth century has considerably furthered our knowledge of substances, although not, as is often implied, by eliminating the macroscopic concepts or reducing macroscopic theory to the theory of atoms, molecules and suchlike. In this paper I will endeavour to show how mereological order can be seen in the way the pioneers of chemistry understood the notion of substance and provides some insight into the ontological implications of their discoveries. The natural continuation of this investigation is to consider how the interplay between micro- and macroscopic concepts in modern chemistry, which seems not to presuppose theoretical reduction,<sup>4</sup> can be understood in mereological terms. But there will not be space to explore this topic here.

This project is conceived in the same spirit that Duhem declared “To give the history of a physical principle is at the same time to make a logical analysis of it”.<sup>5</sup> But such endeavours are usually branded analytic philosophy. Although I am quite happy with this association, it should be quite clear that the present approach is sharply at odds with the ideas of Kripke and Putnam<sup>6</sup> on what they call “natural kinds” that underlie much of the discussion of chemistry in contemporary analytic philosophy. This view has been extensively criticised elsewhere,<sup>7</sup> and I will confine myself here to one central train of thought in this natural kind philosophy that bears on the present theme. According to this doctrine, “water” is a natural kind term which is understood in everyday contexts in terms of water’s manifest or “stereotypical” properties as a colourless, transparent, tasteless,

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<sup>4</sup> Robin Findlay Hendry and Paul Needham, “Le Poidevin on the Reduction of Chemistry”, *British Journal for the Philosophy of Science*, 58 (2007), 339-53.

<sup>5</sup> Pierre Duhem, *La théorie physique: son objet—sa structure*, 2e ed., Marcel Rivière & Cie, Paris, 1914. Trans. by Philip Wiener as *The Aim and Structure of Physical Theory*, Princeton University Press, Princeton, 1954; p. 410 [269].

<sup>6</sup> Saul Kripke, *Naming and Necessity*, Blackwell, Oxford, 1980. Hilary Putnam, *Philosophical Papers*, Vol. 2, Cambridge University Press, Cambridge, 1975, and “Is It Necessary That Water Is H<sub>2</sub>O?” in Lewis Edwin Hahn, ed., *The Philosophy of A. J. Ayer*, Open Court, La Salle, Illinois, 1992; pp. 429-54.

<sup>7</sup> Jaap van Brakel, “The Chemistry of Substances and the Philosophy of Mass Terms”, *Synthese*, 69 (1986), 291-324 and *Philosophy of Chemistry: Between the Manifest and the Scientific Image*, Leuven University Press, Leuven, 2000. Paul Needham, “What is Water?”, *Analysis*, 60 (2000), 13-21 and “Microessentialism: What is the Argument?”, *Noûs*, 45 (2011), 1-21.

thirst-quenching, etc. liquid.<sup>8</sup> But what the term actually refers to is determined by scientific criteria, which may well be unknown to the layman. Some primordial act of ostension picked out a particular quantity of matter which was dubbed “water”, and the general term “water” applies to all and only those quantities of matter that bear the relation of being the *same liquid*<sup>9</sup> to this original sample, as determined by scientific criteria. The scientific criteria are taken to amount to consisting of H<sub>2</sub>O molecules, supposedly justifying the claim that water is H<sub>2</sub>O, which is said to be a statement of identity. An important corollary of this externalist theory of the meaning of natural terms is that although the stereotypical properties associated with the term may change over time, the meaning of the term is its extension, i.e. the set of all and only those quantities of matter that the term applies to, which is fixed by the scientific criteria and doesn’t change with time. “Water”, according to this theory, means the same for us now as it did in Aristotle’s time.

Now if water is the chemical substance with the composition determined by the compositional formula H<sub>2</sub>O (leaving aside the question of microstructure) then the sameness relation governing, according to scientific criteria, whether any quantity of matter is the same substance as a given quantity of water is not confined to being the same liquid. In modern chemistry, the possession of a substance property is, in general, independent of phase. As we will see, this became clear shortly after Lavoisier’s innovations. But earlier, perhaps in Joseph Black’s understanding of latent heat, which Lavoisier sought to accommodate, and certainly if we go back to Aristotle, water was understood to be specifically liquid, and water vapour (steam) and ice were taken to be different substances. So the proper understanding of latent heat brought with it a change in the extension of “water”, which has therefore not always had the same meaning in accordance with scientific criteria as Kripke and Putnam would have it. Even if Aristotle has been corrected on this latter point, he was clear that the basic question determining sameness of substance is whether a given quantity of matter comprises one substance or several. Once quantities comprising single substances are isolated, their distinguishing features can be determined. This fundamental insight was retained even though the phase-dependent conception of substance finds no place in the thermodynamic conception of mixture, and is a further point on which the Kripke-Putnam view errs.

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<sup>8</sup> Putnam *op. cit.* (fn 6), 1975, p. 269.

<sup>9</sup> Putnam *op. cit.* (fn 6), 1975, p. 225.



The general plan of this essay is to first describe in a little more detail the important historical developments in the concept of chemical substance outlined above up to the beginnings of chemical thermodynamics. Mereological ideas are then introduced in order to provide analytic interpretations of the Aristotelian conception of substance and mixture and the contrasting Stoic and Lavoisian conceptions. How these ideas should be modified in the light of more recent chemical theory must be left for another paper.

## 1. Aristotle: The Father of Chemistry

Aristotle (384–322 B.C.) is called the father of biology. The scientific revolution culminating in physics in the 17th century had to prove Aristotelian physics wrong. His writings on the concept of chemical substance, though not a term he used, lead me to think that Duhem<sup>10</sup> was right in crediting him with initiating an important tradition in the history of the subject, meriting the title of the father of chemistry.

Aristotle's thought is often acknowledged as a prime force in the development of alchemy, which is now seen as the antecedent of modern chemistry. The question is whether the mysticism associated with alchemy and identified as the aspect of medieval and renaissance alchemy which modern chemistry had to reject should be ascribed to Aristotle. This seems to be the view of Robert Siegfried, who paints a picture of Aristotle as something of a mystic in his history of modern chemistry:

the atomic theory of Democritus lost out in antiquity [to Aristotle's compositional view] because its materialism left no room for the spiritual. The so-called elements of this story were not the material ones of today, but metaphysical causes of the properties of the various bodies experienced.<sup>11</sup>

But although it is true that Aristotelian ideas about the concept of substance had to be overcome in the development of the modern conception of chemical substance, they weren't ideas of a non-material conception of substance, whatever that might be, but ideas of which even Lavoisier, as we will see, couldn't entirely divest himself. Mysticism plays

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<sup>10</sup> Pierre Duhem, *Le mixte et la combinaison chimique: Essai sur l'évolution d'une idée*, C. Naud, Paris, 1902. Translated in *Mixture and Chemical Combination, and Related Essays*, by Paul Needham, Kluwer, Dordrecht, 2002.

<sup>11</sup> Robert Siegfried, *From Elements to Atoms: A History of Chemical Composition*, American Philosophical Society, Philadelphia, 2002; pp. 2-3.

no part in Duhem's account of Aristotle's contribution to the subject, and will not feature in what is said here.

Aristotle distinguished elements and compounds. His word for what is often translated as "compound" describes the result of a mixing process. But he made no distinction between what, on the basis of the criterion provided by the law of definite proportions early in the nineteenth century, came to be called compounds and solutions. I follow Duhem's use of the antiquated medieval term "mixt" as a technical device for referring to the Aristotelian notion without misleading suggestions for the modern reader. Aristotle doesn't assume a distinction between elements and mixts from the outset, however, but introduces a concept of elementary substance as his discussion develops. His starting point is the observation that there are many substances that are transformed into other substances as they interact. The general problem Aristotle addressed first was how to determine whether a given quantity of matter comprises one or more substances. The key to the question, he thought, was homogeneity. He clearly states that all substances (elements and compounds) are homogeneous, or as he puts it, homoeomerous—comprise like parts: "if combination has taken place, the compound *must* be uniform—any part of such a compound is the same as the whole, just as any part of water is water".<sup>12</sup> This is just homogeneity because Aristotle simply took it to be evident that parthood is spatial parthood—a point the Stoics, as we will see, were to dispute.

He doesn't give such a nice crisp statement of the converse claim, that homogeneous matter comprises a single substance. But he seems to take it for granted that what he evidently took to be a quantity of homogeneous matter, e.g. a quantity of bone, is a single substance, and the different homogeneous parts of a heterogeneous quantity of matter, e.g. the flesh, blood and bone in an animal body, are different substances. Thus, when encountering diamond in rock, oil in water and smoke or clouds in air, in each of these cases the first claim tells us that there is more than one substance and the second that there are two. Even when an oil and water mixture is shaken and the oil doesn't form a connected body, the oil droplets naturally coalesce when they come into contact, and when left would eventually form a single uniform layer. Proper mixing or mixt

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<sup>12</sup> DG I.10, 328<sup>a</sup>10f. DG abbreviates *De Generatione et Corruptione*. "I.10" indicates book I, chapter 10, and "328<sup>a</sup>10" is a reference to the line number given in Bekker's edition of Aristotle's works, which is retained in subsequent editions. All quotations from Aristotle are from *The Complete Works of Aristotle*, ed. Jonathan Barnes, Vol. 1, Princeton University Press, Princeton 1984, unless otherwise indicated.

formation, then, is a process involving two or more substances being brought together and resulting in homogeneous matter, which by his criterion is a single substance—a new substance arising from the reaction of the initial ingredients, different in kind from either of them.

Contraposition of the first claim (that heterogeneity marks a distinction of substance) led him to introduce a special kind of “mixing” process to account for changes like that of water from the liquid to the gas. This kind of mixing is an “overwhelming” process in which one ingredient is present in such a large excess that it isn’t itself changed, but completely converts the other ingredient into the same kind as itself. It is introduced in *DG* I.10 alongside proper mixing (described below), and is later applied in *DG* II.4 (after the notion of an element had been introduced) as the mechanism for what he regards as the transmutation of elements, when, for example, water evaporates and becomes what he regarded as the distinct substance, air. So changes known to modern science as phase changes are treated by Aristotle as transmutations of substance. Something like the Aristotelian conception of substances remains in modern chemistry in the use of kind terms like “quartz”, which describes the substance silicon dioxide in a particular solid phase, or “diamond”, which describes the substance carbon in a particular solid phase, distinct from that exhibited by graphite. The term “water” is still often used in this phase-bound sense, which is defined in the *Shorter Oxford English Dictionary* as “the liquid ... which forms the main constituent of seas, lakes, rivers and rain ...”. In this sense, the content of lakes changes to a different substance, ice, when they freeze, and it is not true that all H<sub>2</sub>O is water.

Aristotle distinguished elements and mixts. His predecessors also spoke of elements, but it was Aristotle who systematically introduced the term in relation to mixts, as we will see when discussing his understanding of the mixing process. For the moment, we simply ask, if homogeneity is the characteristic of a single substance, what further feature distinguishes elements from mixts? Aristotle called elements simple substances, by which he meant that

An element ... is a body into which other bodies may be analysed, present in them potentially or in actuality (which of these is still disputable), and not itself divisible into bodies different in form. That, or something like it, is what all men in every case mean by element.<sup>13</sup>

Note what a striking resemblance this definition of an element bears to Lavoisier’s:

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<sup>13</sup> *De Caelo* III.3, 302<sup>a</sup>15ff.

... if, by the term *elements*, we mean to express those simple and indivisible atoms of which matter is composed, it is extremely probable we know nothing at all about them; but if we apply the term *elements*, or *principles of bodies*, to express our idea of the last point which analysis is capable of reaching, we must admit, as elements, all the substances into which we are capable, by any means, to reduce bodies by decomposition.<sup>14</sup>

In addition to agreeing that no help is to be had by resorting to the doctrine of atomism, they shared a compositional conception of substance according to which the elements are special cases that are not composed of any distinct kind of substance. Lavoisier was able to make much greater use of the notion, however, by taking advantage of Newton's conception of mass and supplementing the analytical idea with a criterion of decomposition in the form of the law of the conservation of mass. This gave an experimental pointer to when a decomposition into simpler parts had actually occurred, which he famously put to use in demolishing the phlogiston theory by determining that a metal rather than the calx produced by calcination of the metal in air is the simpler substance. Aristotle didn't have the notion of mass.

Lavoisier expressed the metaphysical principle underlying the conservation of mass as follows:

We may lay it down as an incontestible [*sic.*] axiom, that, in all the operations of art and nature, nothing is created; an equal quantity of matter exists both before and after the experiment ...<sup>15</sup>

As we will see, there is good reason to think that Aristotle presupposed the same metaphysical principle that matter itself is neither created nor destroyed. But a clear difference emerges as Lavoisier continues this last passage:

the quality and quantity of the elements remain precisely the same; and nothing takes place beyond changes and modifications in the combination of these elements. ... We must always suppose an exact equality between the elements of the body examined and those of the products of its analysis.<sup>16</sup>

Whereas Lavoisier thought that the elements are permanent features of matter that are preserved even when combined in compounds, Aristotle, as

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<sup>14</sup> Antoine Lavoisier, *Traité élémentaire de Chimie*, Paris, 1789. Trans. by Robert Kerr as *Elements of Chemistry*, Dover reprint, New York, 1965; p. xxiv.

<sup>15</sup> Lavoisier *op. cit.* (fn. 14), p. 130.

<sup>16</sup> Lavoisier *op. cit.* (fn. 14), pp. 130-1.

we have seen, didn't think so. Not only did he hold that the elements were subject to transmutation in processes we would understand as phase changes, but he also maintained that the original substances that go to form a proper mixt are not actually present in the mixt. It may have been a disputable question at the point where he introduces the above definition of an element in *De Caelo*, but he settles the point in favour of the interpretation of elements as only potentially present in a mixt. They are there potentially in the sense that they can, in principle, be obtained by a process of decomposition, but are not actually present in the sense that no part of the matter comprising the mixt is an element. This is a natural consequence of his understanding of the way the properties of the elements drive the process of mixt formation.

In the final chapters of Bk I of *DG*, Aristotle describes how matter enters into mixing processes in virtue of capacities and susceptibilities for interaction with other matter, which comes down to the interplay of contraries conferring the ability to act or be acted upon. Contrary properties correspond to different degrees over a range of some determinable, and two quantities of matter bearing contrary properties might be expected to interact with the net result that some intermediate degree of the same determinable is realised by the entire matter comprising the original ingredients. As he later summarised it,

since there are differences in degree in hot and cold, ... [when] both by combining destroy one another's excesses so that there exist instead a hot which (for a hot) is cold and a cold which (for a cold) is hot; then there will exist ... an intermediate. ... It is thus, then, ... that out of the elements there come-to-be flesh and bones and the like—the hot becoming cold and the cold becoming hot when they have been brought to the mean. For at the mean is neither hot nor cold. The mean, however, is of considerable extent and not indivisible. Similarly, it is in virtue of a mean condition that the dry and the moist and the rest produce flesh and bone and the remaining compounds.<sup>17</sup>

With the neutralisation of all such contrary properties of the original ingredients, all their qualitative differences are obliterated and the resulting mixt is a homogeneous quantity with no trace of any physical discontinuity by which the original substances might be distinguished. But, as mentioned above, mixt formation is not the only possible result of the interplay of contraries that Aristotle envisages. Only when the quantities of interacting matter are of “comparable” amounts does a mixt result. Otherwise, when one of the ingredients is present in a much larger

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<sup>17</sup> *DG* II.7, 334<sup>b</sup>8–30.

amount, the contraries of the larger quantity so overwhelm those of the other that the result is a quantity of matter which bears the contraries initially born by the larger quantity without any remission of degree. The obvious questions about which measurable magnitude determines the amounts at issue and how to draw a boundary between “comparable” and “overwhelming” amounts seem to receive no answer in *DG* or anywhere else in Aristotle’s extant works.

The conception of mixing described in *DG* I.10 makes no appeal to the notion of an element, presupposing only that any mixt can be considered to be the result of mixing some other substances. Elements are subsequently introduced in book II, which in agreement with his predecessor Empedocles, Aristotle names as Fire, Water, Air, and Earth. But rather than simply assuming the elements were four in number, Aristotle provided a general characterisation distinguishing elements from other substances and claimed to prove there are just four from more fundamental principles deriving from the forces that induce bodies to mix.

When brought into contact, substances interact in virtue of the mutual powers and susceptibilities conferred by properties, which he argues in *DG* II.2, can be reduced to degrees of warmth and humidity. There are maximal and minimal “contrary extremes”<sup>18</sup> of each of these two fundamental scales, hot and cold being the extremes of warmth, moist and dry those of humidity, and elements are substances with these extremal properties. Since “it is impossible for the same thing to be hot and cold, or moist and dry ... Fire is hot and dry, whereas Air is hot and moist ...; and Water is cold and moist, while Earth is cold and dry”.<sup>19</sup> Accordingly, there are just four elements. The assumption that the primary determinables of warmth and humidity are bounded above and below goes beyond the assumption of the existence of mixed substances (resulting from the mixing of other substances) and provides for the introduction of a general concept of an element. It is a postulate ensuring that there are substances from which all compounds can be considered to be made. (The existential quantifier here stands outside the scope of the universal quantifier. Russell famously illustrated the logical point at issue by pointing out that although all men have a father, it doesn’t follow from this that there is a father of every man.) There are no degrees of the primary determinables outside these limits that could characterise substances that would generate these ingredients from which all other substances are in fact made upon mixing.

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<sup>18</sup> *DG* II.8, 335<sup>a</sup>8

<sup>19</sup> *DG* II.3, 330<sup>a</sup>30–330<sup>b</sup>5.

When he goes on in *DG* II.3 to agree with “all who make the simple bodies elements”,<sup>20</sup> Aristotle has in effect given “simple” the sense of “not generated by mixing other substances”. Speaking in this way of what is generated by mixing gives what might be called the synthetic sense of simplicity, in contrast with the analytic notion described in the passage quoted above from *De caelo* III.3.

An account of simplicity in terms of possessing “a principle of movement in their own nature”<sup>21</sup> is elaborated earlier in *De caelo*. How this squares with the notion of simplicity endowed by the contrary extremes of *DG* is not clear from Aristotle’s extant texts. There is also the problem of understanding how it is that there are many mixts, despite “All the compound bodies ... [being] composed of all the simple bodies”.<sup>22</sup> There are hints that he understood this in terms of being generated by mixing different proportions of elements, but this is problematic. Proportions of elements in compounds have been understood since Lavoisier on the basis of the concept of mass. But this wasn’t available to Aristotle, whose conception of proportion must have some other basis.<sup>23</sup> I turn now to the issue raised in the *De caelo* definition of whether elements are “present in them [other bodies] potentially or in actuality”.

## 2. The Stoic Alternative to Potential Presence

The elements are not actually present in mixts, according to Aristotle. Mixing is driven by the powers to affect and susceptibilities to be affected of the initial ingredients, which change when these powers have run their course and a new substance is formed. In accordance with the homogeneity requirement, that “if combination has taken place, the compound must be uniform—any part of such a compound is the same as the whole, just as any part of water is water”,<sup>24</sup> every part of a mixt has the same intermediate degrees of the qualities characterising the initial ingredients. There are thus no parts with properties characteristic of the elements, namely the extremes of warmth and humidity, and elements are nowhere to be found in a mixt. But although not actually present, Aristotle

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<sup>20</sup> *DG* II.3, 330<sup>b</sup>7.

<sup>21</sup> 268<sup>b</sup>28.

<sup>22</sup> *DG* II.8, 334<sup>b</sup>31.

<sup>23</sup> A line of speculation on this issue is developed in Paul Needham, “An Aristotelian Theory of Chemical Substance”, *Logical Analysis and History of Philosophy*, 12 (2009), 149–64.

<sup>24</sup> *DG* I.10, 328a10f.

says that they are potentially present in the sense that they are potentially recoverable.

Whilst the neutralisation of the characteristic elemental properties when brought into contact by the attainment of intermediate degrees of warmth and humidity is intuitively understandable, it is difficult to understand what, on Aristotle's view, drives the generation of elements by decomposition of a mixt. Perhaps the introduction of the second, overwhelming, kind of mixing was intended to address this problem. But we might sympathise with the Stoics who sought a view of mixts that made decomposition into elements more readily intelligible.

The Stoics distinguished two kinds of mixt. One results from a mixing process that Chrysippus, according to Alexander of Aphrodisias, called "total fusion with both the substances and their qualities being destroyed together". This, Alexander continues, he "says happens with medical drugs in the joint-destruction of the constituents and the production of some other body from them".<sup>25</sup> Fusions are homogeneous, like Aristotle's mixts, but differ from them in being indecomposable. Blends, on the other hand, are also like Aristotelian mixts in being homogeneous, but unlike fusions, their original ingredients are separable because they are actually present in the blend. Stobaeus gives the example of the separation of water from wine: "That the qualities of blended constituents persist in such blendings is quite evident from the fact that they are frequently separated from one another artificially. If one dips an oiled sponge into the wine which has been blended with water, it will separate the water from the wine since the water runs up into the sponge".<sup>26</sup>

The apparent conflict between the requirements of homogeneity and actual presence of the elements in a blend is avoided by rejecting Aristotle's view that two quantities of matter cannot occupy the same region of space at the same time. The Stoics held that spatial uniformity is consistent with the elements composing a compound occupying the same region as the compound and as one another. Alexander tells us that Chrysippus held that "blending in the strict sense of the term" results in "[t]he mutual coextension of some two or even more bodies in their entirety with one another so that each of them preserves their own substance and its qualities in such a mixture ...; for it is a peculiarity of bodies that have been blended that they can be separated again from one

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<sup>25</sup> 216.14. References in this form are to Robert B. Todd, *Alexander of Aphrodisias on Stoic Physics*, E. J. Brill, Leiden 1976, by the number of the first line of the paragraph from which the quotation is taken.

<sup>26</sup> A. A. Long and D. N. Sedley, *The Hellenistic Philosophers*, Volume 1, Cambridge University Press, Cambridge, 1987; p. 291.



another, and this only occurs through the blended bodies preserving their own natures in the mixture”.<sup>27</sup>

The Stoic view of blends would circumvent the Aristotelian conception of the potential presence of elements in mixts based on the intuition that separation is only possible of what is actually present in the mixt. This may sound quite promising, but it faces the problem of characterising the elements in terms of properties exhibited in *both* isolated and combined states, i.e. to describe their “natures” which are preserved in blends. Aristotle defined the elements by conditions they exhibit in isolation—conditions which nothing in a mixt can satisfy. But this strategy is clearly not available on the Stoic view. The Stoics don’t seem to have been able to meet this challenge.

Alexander doesn’t say what the Stoic view on elements was. Bréhier<sup>28</sup> says that Chrysippus subscribed to the common view of the four elements, intertransmutable as for Aristotle, albeit by a different mechanism.<sup>29</sup> The Stoic view must differ from the Aristotelian view by requiring that features characterising the elements are exhibited in the blended state—an impossibility on the Aristotelian view in so far as blends are homogeneous—to account for the possibility of separation. And this, as Alexander in effect points out, precludes adopting the Aristotelian definitions of the

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<sup>27</sup> 216.14. The possibility of cooccupancy is often rejected out of hand by contemporary analytic philosophers, much as Aristotle did. But it is interesting to note that Duhem was prepared to question what many physicists regarded as the “impossibility that they call the *impenetrability of matter*” (*Traité d’énergétique ou de thermodynamique générale*, Gauthier-Villiers, Paris, 1911, p. 15; see Paul Needham, “Duhem’s Theory of Mixture in the Light of the Stoic Challenge to the Aristotelian Conception”, *Studies in History and Philosophy of Science*, 33 (2002), 685-708 for further quotations and discussion), quite independently of the Stoic doctrine, in the interests of interpreting thermodynamics. Also Laszlo Tisza, *Generalized Thermodynamics*, M.I.T. Press, Cambridge, Mass., 1977, p. 128 comments that the unusual systems involved in Ramsey’s discussion of negative temperature comprise a collection of nuclear spins thermally isolated from the lattice “occupying the same region of space”. Remarking that “two isolated systems (spin and lattice) occupying the same region of space is in conflict with [a definition of his theory of macroscopic thermodynamic equilibrium]”, he acknowledges that “our basic theory is restricted to a narrower class of systems, in order to yield a larger number of theorems. However, the procedure is consistent with the use of different definitions to suit specialized situations”. For further remarks on the possibility of cooccupancy, see Paul Needham, “Macroscopic Mixtures”, *Journal of Philosophy*, 104 (2007), 26-52; pp. 41-2.

<sup>28</sup> Émile Bréhier, *Chrysippe et l’ancien stoïcisme*, 2nd. ed., Presses Universitaires de France, Paris, 1951; Ch. II, §2.

<sup>29</sup> Bréhier *op. cit.*, pp. 138-9.

elements on the Stoic view. For “how could anyone say that there is something actually hot in what is cold?”<sup>30</sup> Some ancient sources suggest each element was defined by just one of the four primary qualities Hot (fire), Cold (air), etc.<sup>31</sup> But this doesn’t avoid the problem of contraries in the same place. Hahm<sup>32</sup> suggests that the elements were characterised by differences in density. But this would mean that the elemental properties are not preserved in a blend, since a quantity would occupy a greater volume when part of a blend compared with the isolated state.

Aristotle meets the problem of mixture in so far as he proposes that elements have properties which explain how they interact (effect one another) and produce something with different properties by the straightforward (if naive) device of saying that the resultant matter has degrees of the determinables in question intermediate between those of the interacting elements. Their not being present in the compound doesn’t prevent them interacting to generate the compound in this way. But as indicated above, the process of decomposition of a mixt into elements is not as readily understandable as Aristotle’s account of mixt formation. And as empirical theories, neither kind of process seems particularly well founded. But on the general issue of principle, Aristotle has a coherent conception of elements and their relation to substances formed from them, whereas the Stoic theory doesn’t seem to have a concept of element appropriate to it.

### 3. Beginnings of Modern Chemistry

Modern physics got off the ground in the 17th century with Newtonian mechanics, where matter is characterised with the universal property of mass. Aristotelian physics related the way different bodies move to their different chemical constitution, but Galileo and then Newton removed the distinctions of substance from the mechanics of motion. There was therefore no role for chemistry, concerned as it was with the distinction of kinds of substance, in the physics of the scientific revolution. But after Lavoisier incorporated the notion of mass at the end of the 18th century, chemistry finally became properly integrated with physics in the second half of 19th century with the development of thermodynamics, which recognises a division of the mass into amounts of different substances.

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<sup>30</sup> 224.22.

<sup>31</sup> Bréhier *op. cit.*, p. 136.

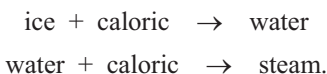
<sup>32</sup> David E. Hahm, “The Stoic Theory of Change”, *Southern Journal of Philosophy*, 13 (supplement) (1985), 39–56; pp. 42ff.

Thermodynamics also treats substance and phase independently, which Aristotle didn't, and it is interesting to note some points in the development of the notion of chemical substance after the advent of Newtonian mechanics leading up to the establishment of this distinction.

In 1761 Joseph Black discovered that heating a body doesn't always raise its temperature. In particular, he noticed that heating ice at 0°C converts it to liquid at the same temperature. Similarly, there is a latent heat of vaporisation that must be supplied for the conversion of a liquid into steam at the boiling point without raising the temperature. He had shown that heat must be distinguished from the state of warmth of a body and even from the changes in that state. But it was some time before the modern interpretation of Black's groundbreaking discovery was fully developed. Theories of heat as a substance in its own right were common at the time and Black was familiar with them, although it was Lavoisier who was to coin the term "caloric" for the heat substance. Black seems to have thought that what we would call the phase changes when ice melts and liquid water boils involve a combination of one substance with the heat substance. Thus, describing an experiment in which water is boiled, he says

The water that remained could not be hotter than the boiling-point, nor could the vessel be hotter, otherwise it would have heated the water, and converted it into vapour. The heat, therefore, did not escape along with the vapour [on opening a valve], but *in* it, probably united to every particle, as one of the ingredients of its vaporous constitution. And as ice, united with a certain quantity of heat, is water, so water, united with another quantity of heat, is steam or vapour.<sup>33</sup>

Black evidently thought that supplying latent heat involved chemical reactions which, using Lavoisier's term "caloric", might be represented by



Only free caloric, uncombined with any other substance, leads to the increase in a body's degree of warmth as it accumulates. This shows that Black was still in the grip of the Aristotelian conception of substance as necessarily connected with a certain phase: to change the phase is to change the substance.

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<sup>33</sup> Quoted by Douglas McKie and Niels H. de V. Heathcote, *The Discovery of Specific and Latent Heats*, Edward Arnold, London, 1935, reprinted by Arno Press, New York, 1975; pp. 23-4.

Lavoisier took over this understanding of substances lock, stock and barrel, his reprimanding Aristotle's doctrine of the four elements notwithstanding.<sup>34</sup> He even retains one of the Aristotelian elements, listing caloric as the "element of heat or fire".<sup>35</sup> This element "becomes fixed in bodies ... [and] acts upon them with a repulsive force, from which, or from its accumulation in bodies to a greater or lesser degree, the transformation of solids into fluids, and of fluids to aeriform elasticity, is entirely owing".<sup>36</sup> He goes on to define *gas* as "this aeriform state of bodies produced by a sufficient accumulation of caloric". Under the list of binary compounds formed with hydrogen, caloric is said to yield hydrogen gas,<sup>37</sup> and he says that hydrogen is the base of hydrogen gas. Similarly, under the list of binary compounds formed with oxygen, caloric yields oxygen gas,<sup>38</sup> and with phosphorus yields phosphorus gas.<sup>39</sup>

In other respects, Lavoisier's list of elements departs radically from the Aristotelian four. Although fire, in the form of caloric, remains, air is analysed into components. During the calcination of mercury, "air is decomposed, and the base of its respirable part is fixed and combined with the mercury ... But ... [a]s the calcination lasts during several days, the disengagement of caloric and light ... [is] not ... perceptible".<sup>40</sup> The base of the respirable part is called oxygen, that of the remainder azote or nitrogen.<sup>41</sup> Thus, oxygen is the base of oxygen gas, and is what combines with caloric to form the compound, which is the gas.

Water is famously demonstrated to be a compound of hydrogen and oxygen in a series of experiments, involving both analysis and synthesis, designed to jointly exclude any other interpretation.<sup>42</sup> The last of these is mentioned here, illustrating the crucial principle involved in this interpretation of the facts:

When 16 ounces of alcohol are burnt in an apparatus properly adapted for collecting all the water disengaged during the combustion, we obtain from 17 to 18 ounces of water. As no substance can furnish a product larger than its original bulk, it follows, that something else has united with the alcohol during its combustion; and I have already shown that this must be

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<sup>34</sup> Lavoisier *op. cit.* (fn. 14), p. xxiii.

<sup>35</sup> Lavoisier *op. cit.* (fn. 14), p. 175.

<sup>36</sup> Lavoisier *op. cit.*, (fn. 14) p. 183.

<sup>37</sup> Lavoisier *op. cit.* (fn. 14), p. 198.

<sup>38</sup> Lavoisier *op. cit.* (fn. 14), p. 190.

<sup>39</sup> Lavoisier *op. cit.* (fn. 14), p. 204.

<sup>40</sup> Lavoisier *op. cit.* (fn. 14), p. 38.

<sup>41</sup> Lavoisier *op. cit.* (fn. 14), pp. 51-3.

<sup>42</sup> Lavoisier *op. cit.* (fn. 14), pp. 83-96.

oxygen, or the base of air. Thus alcohol contains hydrogen, which is one of the elements of water; and the atmospheric air contains oxygen, which is the other element necessary to the composition of water.<sup>43</sup>

The metaphysical principle of the conservation of matter—that matter can be neither created nor destroyed in chemical processes—called upon here is at least as old as Aristotle. What the present passage illustrates is the employment of a criterion of conservation—the preservation of mass. The total mass of the products must come from the mass of the reactants, and if this is not to be found in the easily visible ones, then there must be other, less readily visible reactants. This certainly wasn't the operational criterion it is often billed as being. Although the weightless caloric doesn't conflict with the criterion, it is certainly not identified by virtue of the criterion. Light also figures in his list of elements, being said “to have a great affinity with oxygen ... and contributes along with caloric to change it into the state of gas”.<sup>44</sup> Like caloric, it too is without weight, but Lavoisier saw no obstacle in the criterion of decomposition to the introduction of elements that had a role to play in his scheme.

#### 4. A Mereological Interpretation of these Views

Mereology is a simple algebraic theory that can be formulated in several equivalent ways. Here I choose the variables  $\pi, \rho, \sigma \dots$  to range over quantities of matter and take as primitive the relation of separation, symbolised by “|”. The sentence  $\pi | \rho$  is interpreted intuitively to say that  $\pi$  and  $\rho$  have no part in common. The relations of part, “ $\subseteq$ ”, proper part, “ $\subset$ ” and overlapping, “ $\circ$ ”, are defined as follows:

$$D1 \quad \pi \subseteq \rho \equiv \forall \sigma (\sigma | \rho \supset \sigma | \pi)$$

$$D2 \quad \pi \subset \rho \equiv . \pi \subseteq \rho \wedge \pi \neq \rho$$

$$D3 \quad \pi \circ \rho \equiv \exists \sigma (\sigma \subseteq \pi \wedge \sigma \subseteq \rho).$$

The symbol  $\forall$  in D1 is the universal quantifier and  $\forall \sigma (\sigma | \rho \supset \sigma | \pi)$  is read “for all  $\sigma$ , if  $\sigma | \rho$  then  $\sigma | \pi$ ”, the symbol “ $\supset$ ” standing for implication. Similarly in D2 and D3, the symbol “ $\wedge$ ” stands for conjunction, and  $\pi \subseteq \rho \wedge \pi \neq \rho$ , for example, is read “ $\pi \subseteq \rho$  and  $\pi \neq \rho$ ”. The symbol  $\exists$  in D3 is the existential quantifier and  $\exists \sigma (\sigma \subseteq \pi \wedge \sigma \subseteq \rho)$  in D3 is read “for some  $\sigma$ ,  $\sigma | \rho$  and  $\sigma | \pi$ ”. On the basis of the classical

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<sup>43</sup> Lavoisier *op. cit.* (fn. 14), p. 96.

<sup>44</sup> Lavoisier *op. cit.* (fn. 14), p. 185.

logical principles for the sentential connectives “ $\sim$ ” (not), “ $\vee$ ” (or), “ $\supset$ ” (if ... then ...), etc., the existential and universal quantifiers and the identity relation, the first-order theory of mereology is then formulated by laying down three axioms. First, an identity condition is specified by:

$$\text{M1} \quad \rho \subseteq \pi \wedge \pi \subseteq \rho \supset \rho = \pi.$$

A further axiom suffices to yield the usual connections between the mereological relations:

$$\text{M2} \quad \rho \bullet \pi \equiv \sim(\rho \mid \pi).$$

Finally, an *existential* axiom schema provides for the existence of sums:

$$\text{M3} \quad \exists \pi \varphi(\pi) \supset \exists \rho \forall \sigma (\sigma \mid \rho \equiv \forall \pi (\varphi(\pi) \supset \sigma \mid \pi)).$$

Uniqueness of sums follows from the other axioms, permitting the definition of the sum of quantities  $\pi$  with the property  $\varphi$ ,  $\sum \pi \varphi(\pi)$ , or the sum of  $\varphi$ -ers for short, as follows:

$$\text{D4} \quad \exists \pi \varphi(\pi) \supset . \sigma = \sum \pi \varphi(\pi) \equiv \forall \rho (\rho \mid \sigma \equiv \forall \pi (\varphi(\pi) \supset \rho \mid \pi)).$$

The binary sum,  $\pi \cup \rho$ , is defined as the sum of quantities with the property of being identical either with  $\pi$  or with  $\rho$ . Since there is no null element in mereology as there is in Boolean algebra, it is necessary to guard against forming a sum of  $\varphi$ -ers where  $\varphi$  is a property not satisfied by any object, such as the property of not being self-identical. This is why the existential axiom M3 and the definition D4 are conditional on the condition  $\exists \pi \varphi(\pi)$ .

This axiomatisation neatly distinguishes between the mereological relations and the mereological operations, product and difference being definable in terms of the sum operation. These standard mereological notions can be supplemented with a few other basic concepts suitable for representing the basic ideas of the Aristotelian and Stoic notions of mixture.

The Aristotelian theory serves as a basis for the introduction of a number of *substance properties*,  $S_1, S_2, \dots$  by a procedure described below. These are two-place relations,  $S_i(\pi, t)$ , relating a quantity of matter and a time. The time dependence arises because substances undergo change into other substances via mixing processes. This holds as much for elementary substances as for mixts because on the Aristotelian theory, even the elements undergo transmutation into other elements as well as

into mixts. They all satisfy the condition of applying to all the parts of whatever they apply to:

$$(1) \quad S_i(\pi, t) \wedge \rho \subseteq \pi \wedge t' \subseteq t \rightarrow S_i(\rho, t').$$

Here I have assumed that times are extended intervals, which enter into mereological relations.<sup>45</sup> In the theory of mass terms, (1) is called the *distributive condition*, where it is complemented with a cumulative condition roughly to the effect that the property in question applies to the sum of whatever quantities it applies to.<sup>46</sup> But however natural it might be to associate the cumulative condition with the distributive condition, Aristotle himself seems not to have made the connection.

All substances are characterised in terms of the two transitive and reflexive relations,  $\geq_w$ , of being at least as warm as and  $\geq_h$ , of being at least as humid as, in which they stand to each other and to themselves. These relations change from time to time, however, and should therefore be expressed as three-place, time-dependent relations between two quantities and a time,  $\geq_w(t)$  and  $\geq_h(t)$ . Transitivity and reflexivity are accordingly understood to hold for a fixed time, and expressed as follows:

$$(2) \quad \pi \geq_w(t) \rho \wedge \rho \geq_w(t) \sigma \rightarrow \pi \geq_w(t) \sigma$$

$$(3) \quad \pi \geq_w(t) \rho \supset \pi \geq_w(t) \pi.$$

Given that times are intervals, (2) can be extended to the effect:

$$(2a) \quad \pi \geq_w(t) \rho \wedge \rho \geq_w(t') \sigma \wedge t' \subseteq t \rightarrow \pi \geq_w(t') \sigma.$$

It is natural to assume that these warmth and humidity relations are distributive over time, and also that they hold between all the parts of any quantities between which they hold. In this respect they resemble the intensive character of temperature (and the corresponding relation “at least as warm as”) in equilibrium thermodynamics. Accordingly, any quantity as warm (humid) as itself is uniform in the sense of being as warm (humid) as each of its parts, and so homogeneous (because Aristotle thought phase properties somehow reducible to warmth and humidity). From the modern point of view, equilibrium conditions don’t hold universally. But Aristotle assumes that substance properties are distributive, and that being a particular kind of substance corresponds to having

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<sup>45</sup> For the details of a theory of temporal order bases on mereological principles, see Paul Needham, “Temporal Intervals and Temporal Order”, *Logique et Analyse*, 93 (1981), 49-64.

<sup>46</sup> For details, see Needham *op. cit.* (fn. 27), 2007.

particular degrees of warmth and humidity uniformly. Perhaps material can be in such a condition that its parts are not of definite substance kinds. But for simplicity I assume this is not the case on the Aristotelian view and that the warmth and humidity relations are distributive, in which case the restriction of reflexivity can be dropped and (3) replaced by

$$(4) \quad \pi \geq_w(t) \pi.$$

The relations of “as warm (humid) as” are equivalence relations (for fixed time) when defined by

$$D5 \quad \pi \approx_w(t) \rho \equiv . \pi \geq_w(t) \rho \wedge \pi \leq_w(t) \rho$$

$$D6 \quad \pi \approx_h(t) \rho \equiv . \pi \geq_h(t) \rho \wedge \pi \leq_h(t) \rho,$$

where  $\pi \leq_w(t) \rho$  (for “ $\pi$  is at least as cold as  $\rho$ ”) is just the converse,  $\rho \geq_w(t) \pi$ , and similarly  $\leq_h(t)$  is the converse of  $\geq_h(t)$ . It was Aristotle’s view that particular substances correspond to particular degrees of warmth and humidity. The relation of being the same substance can, accordingly, be defined in this way:

$$D7 \quad \text{SameSubst}(\pi, \rho, t) \equiv . \pi \approx_w(t) \rho \wedge \pi \approx_h(t) \rho.$$

From the fact that  $\approx_w$  and  $\approx_h$  are distributive equivalence relations it follows that for fixed  $t$ , *SameSubst* is also a distributive equivalence relation. Suppose we find a quantity of matter,  $\pi$ , which is a single substance throughout some time  $t$ , i.e. whose every part is the same substance:

$$D8 \quad \text{SingleSubst}(\pi, t) \equiv \forall \rho \forall t' (\rho \subseteq \pi \wedge t' \subseteq t \supset \text{SameSubst}(\pi, \rho, t')).$$

A two-place predicate,  $S_1$ , can now be introduced to describe this substance, and this predicate satisfies condition (1). A quantity comprising a single substance that is not the same substance as a given quantity but nevertheless itself a single substance is a distinct substance:

$$D9 \quad \text{DistSubst}(\pi, \rho, t) \equiv . \sim \text{SameSubst}(\pi, \rho, t) \\ \wedge \text{SingleSubst}(\pi, t) \wedge \text{SingleSubst}(\rho, t).$$

With the aid of some additional principles introduced shortly it will be possible to show that D9 implies that  $\pi$  and  $\rho$  are separate.

A two-place predicate,  $S_2$ , can be introduced to describe a substance distinct from substance  $S_1$ , a further two-place predicate,  $S_3$ , can be



introduced to describe a substance distinct from each substance  $S_1$  and  $S_2$ , and so on for as many substances as can be found, all these predicates satisfying condition (1). This procedure leaves it open to establish characteristic properties of each of these substances, which can be assembled in lists amounting to an alternative means of establishing distinctness of substance when direct mixing is inconvenient. It is in this way that the elements are distinguished from substances in general.

The elements are characterised by having extreme degrees of warmth and humidity. To express this idea, we first have to lay it down that warmth and humidity are bounded above and below:

$$(5) \quad \exists \pi \forall \rho (\pi \geq_w(t) \rho) \wedge \exists \pi \forall \rho (\pi \leq_w(t) \rho),$$

and similarly for  $\geq_h$ . (As it stands, this holds for all times,  $t$ . This is the expression of the principle that the vocabulary introduced so far allows us to formulate. Modifications, including the possibility of accommodating the principle in modal terms, will be considered shortly.) The extremal property of being wet ( $W$ ) can now be defined as being at least as humid as anything:

$$D10 \quad W(\pi, t) \equiv \forall \rho (\pi \geq_h(t) \rho),$$

and similarly, being dry ( $D$ ) is defined as everything being at least as humid, being hot ( $H$ ) as being at least as warm as anything and being cold ( $C$ ) is defined as everything being at least as warm:

$$D11 \quad D(\pi, t) \equiv \forall \rho (\rho \geq_h(t) \pi)$$

$$D12 \quad H(\pi, t) \equiv \forall \rho (\pi \geq_w(t) \rho)$$

$$D13 \quad C(\pi, t) \equiv \forall \rho (\rho \geq_w(t) \pi).$$

The elemental substance property  $Water(\pi, t)$  can then be defined as  $W(\pi, t) \wedge C(\pi, t)$ , and similarly for  $Earth(\pi, t)$ ,  $Air(\pi, t)$  and  $Fire(\pi, t)$  in accordance with Aristotle's definitions. A mixt is a non-elemental substance with non-extremal degrees of warmth and humidity, i.e. a quantity which, at the time in question, is both strictly warmer than something and strictly colder than something else, as well as being strictly more humid than something and strictly less humid than something else.

Further development requires the introduction of an apparatus for referring to spatial regions,  $p, q, r, \dots$ , analogous to that for temporal

intervals.<sup>47</sup> Here we just introduce the predicates  $Occ(\pi, p, t)$  for “ $\pi$  occupies exactly the region  $p$  throughout  $t$ ” and  $A(p, q)$  for “ $p$  abuts  $q$ ” (thinking of regions as retaining their identity over time, as though they are parts of a Newtonian absolute space). A principle common to both Aristotelian and Stoic views is:

$$(6) \quad Occ(\pi, p, t) \wedge Occ(\rho, q, t) \wedge p \mid q \rightarrow \pi \mid \rho.$$

The fundamental Aristotelian principle of the impossibility of cooccupancy can be formulated for stationary quantities as

$$(7a) \quad Occ(\pi, p, t) \wedge Occ(\rho, q, t) \wedge \pi \mid \rho \rightarrow p \mid q.$$

Allowing that  $\pi$  and  $\rho$  might move, sweeping out regions which overlap, a more restricted principle along the lines of

$$(7b) \quad Occ(\pi, p, t) \wedge Occ(\rho, q, t) \wedge \pi \mid \rho \rightarrow \exists p' \subseteq p \exists q' \subseteq q \\ \exists t' \subseteq t (Occ(\pi, p', t') \wedge Occ(\rho, q', t') \wedge p' \mid q').$$

is required to cover the general case. Further, the general principle that different degrees of the same primary determinable of warmth or humidity cannot be instantiated by matter in the same place can be formulated by laying it down that

$$(8a) \quad Occ(\pi, p, t) \wedge Occ(\rho, q, t) \wedge \sim(\pi \approx_w(t) \rho) \rightarrow p \mid q.$$

$$(8b) \quad Occ(\pi, p, t) \wedge Occ(\rho, q, t) \wedge \sim(\pi \approx_h(t) \rho) \rightarrow p \mid q.$$

With these postulates, it is now possible to show that  $DistSubst(\pi, \rho, t)$  implies  $\pi \mid \rho$ . By D9,  $DistSubst(\pi, \rho, t)$  implies  $\sim SameSubst(\pi, \rho, t)$ , which in turn implies that  $\pi$  and  $\rho$  differ either in warmth or humidity. But since  $\pi$  and  $\rho$  are each single substances, their warmth and humidity is uniform, i.e. the same for all of their respective parts. Accordingly, by (8a) and (8b), every part of  $\pi$  occupies a region separate from every part of  $\rho$  and conversely, so by (6) every part of  $\pi$  is separate from every part of  $\rho$ , in which case  $\pi$  and  $\rho$  are themselves separate.

With a view to expressing that the result of Aristotelian mixing is the attainment of uniform degrees of warmth and humidity, we first stipulate that two regions are connected if they either abut or overlap:

$$D14 \quad Con(p, q) \equiv . A(p, q) \vee p \bullet q.$$

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<sup>47</sup> A suitable axiom system can be devised by generalising the system for temporal intervals mentioned in the previous footnote.

Two quantities,  $\pi$  and  $\rho$ , are then said to be connected throughout  $t$ ,  $Con^*(\pi, \rho, t)$ , if they occupy connected regions throughout  $t$ :

$$D15 \quad Con^*(\pi, \rho, t) \equiv \forall t' \subseteq t \exists p \exists q (Occ(\pi, p, t') \wedge Occ(\rho, q, t') \wedge Con(p, q)).$$

That two quantities of matter, which might have had different degrees of warmth and humidity before  $t$ , have the same degrees of warmth and humidity when in contact at  $t$  can now be expressed as the principle:

$$(9) \quad Con^*(\pi, \rho, t) \supset \exists t' \geq t (\pi \approx_w(t') \rho \wedge \pi \approx_h(t') \rho),$$

where  $t' \geq t$  means “ $t'$  is not earlier than  $t$ ”. (A third conjunct,  $\forall t'' (t' \geq t'' \geq t \wedge Con^*(\pi, \rho, t'')) \supset \pi \approx_w(t'') \rho \wedge \pi \approx_h(t'') \rho$ , might well be added within the scope of the existential quantifier.)

The common degrees of warmth and humidity thereby attained could be further specified to be intermediate between the original degrees. But note that this latter comparison involves two times, to the general effect that the sum of  $\pi$  and  $\rho$  is warmer than  $\pi$  at  $t$  than it was at  $t'$ , and the sum of  $\pi$  and  $\rho$  is colder than  $\rho$  at  $t$  than it was at  $t'$ , and similarly for the humidity relation. These relations can be expressed as  $\pi \cup \rho \geq_w(t', t) \pi \wedge t' < t$ , and  $\pi \cup \rho \leq_w(t', t) \rho \wedge t' < t$ , where  $t' < t$  stands for “ $t'$  is earlier than  $t$ ”. The original three-place warmer than relation (expressed with a single time variable) can be defined in terms of the new four-place relation by identifying the two times:

$$D16 \quad \pi \leq_w(t) \rho \equiv \pi \leq_w(t', t) \rho \wedge t' = t.$$

Now that it has been recognised that relational comparison can involve several times, we can return to the question of how the upper and lower bounds of the as warm as and as humid as relations, expressed above by (5), might be elaborated. As it stands, (5) implies that there is always something at least as warm as anything and there is always something as least as cold as anything. This allows that different things exemplify these extremal properties at different times, which is not itself problematic, but it leaves open the question of some sort of uniform standard over time. This idea can be captured by modifying (5) to read

$$(10a) \quad \exists \pi \exists t \forall t' \forall \rho (\pi \geq_w(t, t') \rho) \wedge \exists \pi \exists t \forall t' \forall \rho (\pi \leq_w(t, t') \rho),$$

to the effect that there is something which is at some time as warm (cold) as anything ever is, and similarly  $\geq_h$  for and  $\leq_h$ .

It might be thought that the idea of extremal degrees of the primary determinables is a modal notion—that they are never actually realised, but are only possibilities. (This would capture the claim expressed by some commentators that the Aristotelian elements are ideal notions, never in fact actually exemplified by any matter.) The expression of this idea presents a problem, however. (10a) might be weakened to

$$(10b) \quad \Diamond \exists \pi \exists t \forall t' \forall \rho (\pi \geq_w(t, t') \rho) \wedge \Diamond \exists \pi \exists t \forall t' \forall \rho (\pi \leq_w(t, t') \rho),$$

where  $\Diamond$  is the sentential operator read “it is possible that”. (The principle of the permanence of matter can be extended to the requirement that there never could be more or less matter than there actually is by adopting the Barcan formula as an axiom, corresponding to a single domain in all possible worlds. Similarly for times.) What we want to say is that there might be something that is at some time as warm as anything ever *actually* is (or could be). But what (10b) in fact says is that it is possible that there is something that is at some time as warm as anything ever is (which shouldn’t be read “as anything ever actually is”). This allows that there isn’t actually any upper bound on the as warm as relation, just that there might be. The problem can be addressed by indexing occurrences of variables predicated by the “as warm as” predicate, say by attaching superscripts to the variables thus:  $\pi^1 \leq_w(t, t') \rho^2$ . The intended thought can now be expressed by

$$(10c) \quad \Diamond^1 \exists \pi \exists t \forall t' \forall \rho \Delta^2 (\pi^1 \geq_w(t, t') \rho^2) \wedge \Diamond^1 \exists \pi \exists t \forall t' \forall \rho \Delta^2 (\pi^1 \leq_w(t, t') \rho^2),$$

where  $\Delta^i$  is an expression of actuality governing the  $i$ th position within its scope. Alternatively, a stronger statement can be made by replacing  $\Delta^2$  in (10c) to an expression of necessity,  $\Box^i$ , defined as  $\sim \Diamond^i \sim$ .<sup>48</sup> These

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<sup>48</sup> A formal interpretation can be developed on the basis that  $n$ -place predicates are assigned extensions comprising ordered  $2n$ -tuples, the odd members of which are drawn either from a domain of quantities or a domain of times, and the even members are drawn from a set of possible worlds. Arbitrary sentences hold in a model relative a pair of sequences, the first comprising times or quantities and assigning values to the free variables, the second drawn from the set of possible worlds. A sentence  $\Diamond^1 \Box$  holds in a model relative a sequence pair iff  $\Box$  holds in the model relative a sequence pair like the former in every respect except that the  $i$ th element of the second sequence is replaced by  $w^i$ , for some possible world  $w^i$ . The clause for  $\Delta^1 \Box$  is similar, except that the replacement is made by a fixed element @, interpreted as the actual world.

expressions of modality are not the usual operators, but predicate modifiers which cannot be iterated, and call for a formal theory which cannot be developed here.

s influence underlying elementary particletelian chemistry can be usefully compared with some of the points made in a recent discussion of Aristotle's theory of mixture in *DG* by John Cooper.<sup>49</sup> Cooper opposes his interpretation to that of a certain tradition among commentators going back to Philoponus who interpret Aristotle's claim in *DG* II.8, that "All the compound bodies ... are composed of all the simple bodies",<sup>50</sup> to imply a "total interfusion" view according to which "the smallest bit of my flesh is put together from all the simple bodies".<sup>51</sup> Against this, Cooper wants to allow the possibility that a small bit of flesh "did not derive from any water, but only from some earth",<sup>52</sup> which he maintains is consistent with the requirement of total uniformity of mixts (the distributive condition). Cooper emphasises that a mixt "results from the mutual interaction of finitely small bits of the separate ingredients acting on one another",<sup>53</sup> but nevertheless acquires the common features characteristic of the mixt because "what was earth, say, now comes to have just the same perceptible characteristics as the fire, and/or the air or the water, that it has been mixed with also come to have".<sup>54</sup>

Cooper seeks to maintain the distinction between the Aristotelian and the Stoic views, which the Philoponus interpretation threatens to run together. I would put his point as building on the distinction between a property and what it applies to. The latter I call quantities of matter, which are treated as things bearing different substance properties (being of different kinds of substance) at different times. This provides for distinguishing between what is and isn't preserved when Aristotle says "The compound may *be actually* other than the constituents from which it has resulted; nevertheless each of them may still *be potentially* what it was before they were combined, and both of them may survive undestroyed".<sup>55</sup> What is not destroyed are the quantities of original ingredients which came together to make the mixt, although the original substance kinds cease to

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<sup>49</sup> John Cooper, "A Note on Aristotle on Mixture", in Frans de Haas and Jaap Mansfeld, eds., *Aristotle: On Generation and Corruption Book I*, Symposium Aristotelicum, Oxford University Press, Oxford, 2004; pp. 315-26.

<sup>50</sup> 334<sup>b</sup>31.

<sup>51</sup> Cooper *op. cit.* (fn. 49), p. 325.

<sup>52</sup> Cooper *op. cit.* (fn. 49), p. 325.

<sup>53</sup> Cooper *op. cit.* (fn. 49), p. 323.

<sup>54</sup> Cooper *op. cit.* (fn. 49), p. 322.

<sup>55</sup> *DG* I.10, 323<sup>b</sup>25-27.

apply to these quantities when forming parts of the mixt. Thus, we can speak with Cooper of what was earth and is now a mixt and may later again be an elemental kind, namely a quantity of matter. The quantities of matter themselves are identifiable throughout such transmutations, in accordance with the mereological criterion of identity, and are not interpenetrable.

What seems to me to be an outstanding difficulty with Aristotle's view is his claim that "The constituents, therefore, neither *persist actually*, as body and white persist; nor are they destroyed (either one of them or both), for their potentiality is preserved".<sup>56</sup> As already suggested, what drives the process of decomposition in which this potentiality is realised is not readily understood. Now it is unclear what should induce a particular part to become, say, water even if that quantity was water before mixing since, if the mixt is uniform, it is like all the other parts in respect of the relevant features of warmth and humidity. In virtue of what, then, is the specific potentiality to become water preserved? This problem is comparable to the chief difficulty facing the Stoic view, of providing a characterisation of the "nature" of elements common to the isolated and blended state. Elsewhere, however, Aristotle suggests that it must be possible to derive the elements from "any and every part of flesh",<sup>57</sup> so that the original quantities don't *preserve* the potentiality to become the same element, but each part of the mixt has the potentiality to become any of the elements (under the constraint that decomposition of the entire mixt will result in quantities of the four elements standing in the same proportion as did the original ingredients). So specific quantities of elements don't preserve a potentiality to become the *same* element when in a mixt, just some element.

It does seem to be clear, however, that the Aristotelian view is based on an assumption of the indestructibility of matter which is reflected in the treatment of quantities in the mereological interpretation offered here and in Cooper's use of expressions like "what was earth ... now comes to have the same... characteristics as fire".<sup>58</sup> We saw earlier that Lavoisier was able to take advantage of Newton's conception of mass as a measure of the

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<sup>56</sup> *DG* I.10, 323<sup>b</sup>29-31.

<sup>57</sup> *DG* II.7, 334<sup>a</sup>34.

<sup>58</sup> Recent Aristotelian scholarship such as James A. Weisheipl, "The Concept of Matter in Fourteenth Century Science", in Ernán McMullin, ed., *The Concept of Matter in Greek and Medieval Philosophy*, University of Notre Dame Press, Notre Dame, Indiana, 1963 and David Bostock, "Aristotle on the Transmutation of the Elements in *De Generatione et Corruptione* 1.1-4", *Oxford Studies in Ancient Philosophy*, Vol. XIII, ed. C. C. W. Taylor, Clarendon Press, Oxford, 1995 can also be cited in support of this view.

amount of matter, which wasn't available to Aristotle, and formulate this principle as the law of the conservation of mass. But the underlying metaphysical principle is the same as Aristotle's.<sup>59</sup> They differed on the question of the permanence of the elements, which is not part of Aristotle's scheme. The Stoics' view was closer to Lavoisier's. They entertained a conception of the permanence of the elements involved in the formation of blends in order to explain the possibility of separation (even if they also allowed for the destruction of elements in fusions).

The basic premise of the Stoic view is the possibility of cooccupancy, definable as

$$D17 \quad Coocc(\pi, \rho, t) \equiv \exists p (Occ(\pi, p, t) \wedge Occ(\rho, p, t)).$$

This relation holds trivially where  $\pi = \rho$ , but the contention is that it can hold for distinct, indeed separate,  $\pi$  and  $\rho$ . This could be used to define a blend along the lines of

$$D18 \quad Blend(\pi, \rho, t) \equiv . \pi | \rho \wedge Coocc(\pi, \rho, t) \wedge DistSubst^*(\pi, \rho, t)$$

if we had an account (perhaps implying  $\pi | \rho$ ) of the relation  $DistSubst^*(\pi, \rho, t)$  of  $\pi$  and  $\rho$  being distinct substances throughout  $t$  on the Stoic view. As we have seen, however, it is unclear by what criterion this latter relationship is established on the Stoic view. Heterogeneity was Aristotle's criterion, but that clearly won't do here where it is envisaged that a blend is homogeneous. The elements cannot be defined as Aristotle defined them in terms of contrary extremes of warmth and humidity if it is possible for them to cooccupy a given region in view of Alexander's principle that contrary features cannot be exhibited in the same place at the same time. This principle isn't captured by the distributivity of the warmth and humidity relations as hitherto assumed, but requires a formulation making explicit reference to regions of space along the following lines:

$$(11) \quad Occ(\pi, p, t) \supset \forall q \forall t' \forall \rho (q \subseteq p \wedge t' \subseteq t \wedge Occ(\rho, q, t') \cdot \supset \rho \approx_w(t') \pi \wedge \rho \approx_h(t') \pi).$$

Consequently, two quantities standing in the blend relation would have the same degree of warmth and humidity.

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<sup>59</sup> Compare Henri Poincaré, "Les conceptions nouvelles de la matière", in Henri Bergson, *et al.*, eds., *Le matérialisme actuel*, Flammarion, Paris, 1913, pp. 49-67, who said (p. 65) that Lavoisier "demonstrated the indestructibility of matter by demonstrating the invariability of mass".

Whether the Stoics were able to make any improvement on this position cannot be known from the scant surviving texts. It seems that Lavoisier, who also adopted the conception of the actual presence of elements in their compounds, offered little advance on this issue. Since he doesn't explicitly declare a view on the cooccupancy or otherwise of elements in compounds, his view of for example a binary compound, abbreviated *BinCpd*, can be expressed without reference to cooccupancy as

$$(12) \quad \text{BinCpd}(\pi, t) \equiv \exists \rho \exists \sigma (\text{DistEl}(\rho, \sigma) \wedge \pi = \rho \cup \sigma) \wedge \\ \text{SinglePhase}(\pi, t),$$

where the relation,  $\text{DistEl}(\rho, \sigma)$ , of being distinct elements (which I take it implies  $\rho \mid \sigma$ ) is not time-dependent because the elements are permanent on Lavoisier's view.  $\text{SinglePhase}(\pi, t)$  says that  $\pi$  exhibits a single phase (solid, liquid or gas) throughout  $t$ . Where the phase is liquid or gas, one of the elements fixed in a binary compound has to be caloric, and caloric may even be fixed in solids. In this case, the second element is easily distinguished from imponderable caloric by virtue of having mass. But Lavoisier explicitly cites ammoniac as a binary compound of nitrogen with hydrogen,<sup>60</sup> by which he presumably means base of ammonia (without caloric). In the same vein, he cites water as a binary compound of hydrogen and oxygen,<sup>61</sup> copper / iron pyrites and galena (sulphur with copper / iron and lead,<sup>62</sup> oxide of phosphorus, phosphuret of hydrogen / nitrogen / sulphur,<sup>63</sup> etc. Whether or not he could claim to have isolated these substances, he is clearly claiming they exist as binary compounds of pairs of elements from the list: nitrogen, hydrogen, oxygen, copper, iron, lead, phosphorus and sulphur, excluding caloric. What distinguishes two quantities of matter as being of distinct element kinds when combined in these cases is not so clear. Elements in isolation exhibit capacities and susceptibilities to interact with others that they lose in the combined state, when they possess the potential to exhibit these and other features typical of the isolated state. But Lavoisier's text leaves it as something of a mystery what non-modal properties they actually possess in the combined state. They display relational features of standing in certain proportions by mass to certain elements in specific compounds, and not combining at all with others. Since Aristotle's conception of the potential presence of

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<sup>60</sup> Lavoisier *op. cit.* (fn. 14), p. 194.

<sup>61</sup> Lavoisier *op. cit.* (fn. 14), p. 198.

<sup>62</sup> Lavoisier *op. cit.* (fn. 14), p. 202.

<sup>63</sup> Lavoisier *op. cit.*, (fn. 14) p. 204.



elements in compounds also allows that analysis results in definite proportions of the isolated elements, however, this doesn't provide a substantial difference between the views. Without an account of how the properties of compounds depend on actual non-modal properties exhibited by elements present in compounds, it remains unclear what the force of Lavoisier's claim of the persistence of elements in compounds is supposed to be.

## 5. Final Words

It is, perhaps, unclear whether Lavoisier thought of air as a compound or merely a mixture,<sup>64</sup> and the requirement of definite proportions has not been written into (12). But after Berthollet raised the question of whether chemical combination requires constancy of proportions and the chemical community decided in favour of Proust's law of definite proportions, this requirement was incorporated into the understanding of what a compound is. Some decades later the caloric theory was finally abandoned with the discovery that heat is not conserved, paving the way for what Lavoisier called the base of such-and-such a phase-restricted stuff to be taken as the general notion of substance, free of any restriction to phase. This understanding of substances was clearly represented in Gibbs' notion of a mixture as a quantity of matter comprising one or more phases over which one or more substances are distributed. This admits of the special cases of a single substance exhibiting one, two or three phases (a pure quantity) and of a quantity exhibiting a single phase containing several substances (a solution). The state of such a quantity in the energy representation is governed by a function,  $U(S, V, N_1 \dots N_r)$ , giving the energy as function of the entropy,  $S$ , the volume,  $V$ , and the relative amount of each component substance,  $N_i$ . In general, a quantity of volume  $V$  comprises  $r$  substances,  $r \geq 1$ , naturally understood to be substances actually present in the mixture. In the case  $r = 1$ , Gibbs' phase rule is understood to provide a criterion of purity. But where what Gibbs called the number of independent substances,  $r$ , is greater than 1, questions of interpretation have arisen and it has been suggested that it doesn't represent the actual number of substances present. There is no space to pursue this matter here, but some of the issues raised are discussed within a mereological framework

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<sup>64</sup> He suggests that it is a compound when he says, for example, that during the calcination of mercury, "air is decomposed, and the base of its respirable part is fixed and combined with the mercury" (Lavoisier *op. cit.* (fn. 14), p. 38).

elsewhere.<sup>65</sup> The question of the relation between micro- and macrolevels is broached in this paper. But the real challenge facing this programme is the nature of the mereological relations between macroscopic quantities, subject to the familiar laws of identity, and quantum ontology. A thorough study of this matter will have to be the subject of a new paper.

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<sup>65</sup> Paul Needham, "Substance and Time", *British Journal for the Philosophy of Science*, 61 (2010), 485-512.

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# RELATIONS BETWEEN LEVELS FROM A CHEMICAL PERSPECTIVE

ANNA CIAUNICA-GARROUTY

## Introduction

A popular view nowadays is that the world is structured so that every part of reality is built on and therefore ontologically dependent on a basic micro-level. Being has units: some of it is fundamental, the rest is derivative. The fundamental bottom level consists of fundamental physical entities. Reality's architectonics comprises several *levels of being*. At the lower level are the things of interest to fundamental physics, the quarks, electrons and fields, and their properties. At higher levels are complex objects and their properties. Complex objects are made up of arrangements of objects at lower levels. Only the fundamental bottom level of this building is "maximally" real, while all the other entities inhabiting the remaining levels are at best derivative, if real at all.

One of the perennial questions in the philosophy of sciences concerns inter-levels relations: how exactly are the higher-level entities related to the lower-level ones? Many philosophers take for granted that chemistry has already been reduced to physics. This assumption was so pervasive that it was common to read about "physic/chemical" laws and explanations, as if the reduction of chemistry to physics was complete. (Hendry, Weisberg & Needham 2011) In reality, the situation is not as simple as philosophers might assume.

The question of relations between chemistry and physics is usually presented within a twofold framework. (i) The first part concerns the link between the fundamental bottom level of physical particles and the higher level of elements, atoms and molecules. The important question here is: "Are atomic and molecular species reducible to systems of fundamental particles interacting according to quantum mechanics?" (ii) The second part concerns the relationship between macroscopic descriptions of chemical substances. Here the main question is: "Are chemical substances reducible to molecular species?"

In §1-2 I examine each of these two aspects and focus on the specific relations between two of the closest realms within the layered picture, i.e. molecular chemistry and atomic physics. In §3 I present an alternative view to Ontological Fundamentalism, namely Priority Monism. Indeed, to depict reality as a storied building is one thing. But to carve reality at its ontological joints is quite another. Typically, difficulties start here: explaining how layers are divided, how they connect between themselves and to the fundamental level itself. Even between two allegedly adjacent levels of the fundamentalist building, the ontological tension remains significant.

## **1. Ontological Fundamentalism and Downwards Causation**

Reality, it is widely presumed, is a hierarchy of distinct yet connected levels starting from a fundamental ground floor. Ontological Fundamentalism ([OF] hereafter) is construed as a set consisting of the following three theses:

- (a) The Hierarchy thesis: The universe is stratified into levels.
- (b) The Fundamentality thesis: There is a bottom level, which is fundamental.
- (c) The Primacy thesis: Entities on the fundamental level are primarily real and the rest are at best derivative, if they are real at all. (Schaffer 2003:498)

The possibility of fully reducing chemical theories about atoms and molecules to quantum mechanics has been questioned and it has been pointed out by Bogaard (1978) and Scerri (1991, 1994) that many key chemical concepts such as valence and bonding do not find a natural home in quantum mechanics. The basic idea is that although quantum chemistry can be extremely illuminating, it has not reduced chemistry to physics. However, if one thinks that [OF] is necessarily committed to reductionism (i.e. deriving the higher-level events exclusively from the lower-level events) then Bogaard and Scerri are right. But there are other sophisticated accounts of the inter-level relations that avoid reduction.

Before proceeding with our discussion, some clarification preliminaries are in order. More specifically we need to define the key concepts of “levels”, “physicalism” and “supervenience”.

According to Schaffer, (2003) there are currently four connotations of “levels”, each of which describes a structure and an ordering relation:

- (a) the mereological structure, ordered by the part-whole relation, according to which the objects on the lower levels of the hierarchy compose the objects on the higher levels;
- (b) the supervenience structure, ordered by asymmetric dependencies, according to which everything that happens on the higher levels supervenes on what is occurring on the lower levels;
- (c) the *realization* structure, ordered by functional relations, according to which the instantiations of various properties and relations on the higher levels must be *realized by* instantiations of properties and relations at the lower levels;
- (d) the *nomological*<sup>1</sup> structure, ordered by one-way bridge principles between families of lawfully interrelated properties according to which the laws of nature governing the higher levels are *reducible* to the laws governing the lower levels.

*Physicalism* is the thesis that the world is, in some sense, nothing over and above the physical<sup>2</sup>, and that the chemical is a derivative feature of reality. It is supposed to determine what the fundamental properties of the world are like and to determine how all higher levels of the world relate to such properties. In the now dominant standard view, higher-level derivative items are not *just* arrangements of lower-level basic items. Higher-level objects and properties might be dependent on those at lower-levels, but this dependence is consistent with a measure of autonomy. Thus higher-level properties are said not to be reducible to—in the sense of identifiable with—lower-level properties. However, physicalism clearly states that all higher-level properties of the world are dependent on fundamental physical properties. In other words, physicalism maintains the primacy, in some sense or other, of physical entities, defined in some way or other. Of course, the important question here is: in what sense are molecules ontologically dependent on elementary physical particles?

In contemporary philosophy, *supervenience*<sup>3</sup> can be spelled out in

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<sup>1</sup> In a broad sense, for anything to be a level of any interest and importance in science, it has to introduce “new” causal or nomological relations.

<sup>2</sup> The definition of “physical” is currently an open question. For a detailed discussion see Stoljar (2010). He distinguishes between Object-based approaches and Theory-based approaches in defining the notion of “physical” property or entity.

<sup>3</sup> It was Davidson who introduced the term *supervenience* while talking about the relationship between the mental level and the physical one, but the supervenience dependence applies undoubtedly to the chemical/physical relations too: “(...) Mental characteristics—he writes—are in some sense dependent, or supervenient, on physical characteristics. Such supervenience might be taken to mean that there

various ways, but in the specific context of physicalism it has become standard to formulate it in terms of the duplication of possible worlds  $w^4$ : any world which is a minimal physical duplicate of our world is a duplicate *simpliciter* (Jackson, 1998:12). In other words, “physicalism is true at  $w$  if and only if for any possible world  $w^*$  if  $w^*$  is a physical duplicate of  $w$ , then  $w^*$  is a duplicate of  $w$  simpliciter.” (Stoljar 2010:116)

To put it in a slogan, supervenience says that: “no changes at the chemical level without changes at the physical level”, which means that there is an asymmetric necessitation relation between the fundamental physical properties and all the other remaining properties. Within the [OF] framework, the higher-level of “water” is said to supervene on the lower level of  $H_2O$ , which supervenes on the physical level of electrons and so on until we reach the bottom level of fundamental physical simples, whatever those might be.

There are two major problems with this picture. The first one is that the asymmetry is taken for granted. (van Brakel 1996a; Earley 2008) The taken for granted asymmetry is obvious, for example, in Kim’s work. He argues that chemical kinds and their microphysical compositions (at least, at one level of description) “seem to strongly covary with each other, and yet it is true, presumably, that natural kinds are asymmetrically dependent on microphysical structures. Here our mereological intuition, that macrophysical properties are asymmetrically dependent on microphysical structures, seems to be the major influence on our thinking, cancelling out the fact that the converse strong covariance may also be present.” (1990:14) Kim holds that all non-reductive versions of physicalism imply “downward causation”, (Kim 2005) i.e. the idea that higher-level properties influence underlying elementary particle-level properties, but he claims that no convincing explanation has yet been offered of how upper-level properties or entities might possibly have effects on lower-level events or individuals. In spite of this pessimistic attitude, some philosophers of chemistry have convincingly argued that chemical properties may constrain the behavior of physical systems. Robin Hendry (2006b) for instance, has considered the possibility of downward causation in quantum-chemical accounts of chemical bonding in molecules. Hendry points out that, in such calculations, the gross molecular structure (atomic connectivity) is generally not a result of quantum-chemical calculations but is put in as an initial assumption based on chemical experience—and that no evidence or argument shows how to avoid invalidating the

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cannot be two events alike in all physical respects but differing in some mental respects. (...)” (1970: 214)

<sup>4</sup> (cf. Lewis 1983; Horgan 1983; Jackson 1998)



reductionist project by making such assumptions. Hendry reaches the conclusion that with respect to its attempt to demonstrate that downward causation does not occur in chemistry, “strict physicalism fails, because it misrepresents the details of physical explanation”.

Here is an example of “downward causation” in a well-understood chemical system given by Earley:

The closure of networks of (upper-level) relationships in open systems of nonlinear chemical reactions gives rise to sustained oscillations that dramatically change effective concentrations of chemical components—the same components that are the active participants in the reactions that are combined. These effects are formally analogous to biological examples (such as the dancing birds) in which upper-level coherence influences lower-level entities. The mathematics that describes those chemical systems is similar to formalisms that represent the biological examples, but the chemical cases are more amenable to quantitative modeling. Quantitative modeling of complex networks of time-dependent chemical processes should be able to clarify conditions in which ‘downward causation’ may be shown to operate on the chemical level—and thereby earn whatever reward may be on offer for meeting Kim’s Challenge. (Earley, 2008:19)

The second problem with the [OF] picture concerns the part-whole relation underlying its ontological commitments. As van Brakel (1996a) pointed out, “mainstream supervenience discussions, although claiming to be in the business of developing a form of non-reductive materialism, are wedded to the intuition of a microreductionistic image of the world.” This leads us to the second part of this paper treating the macroscopic-microscopic intertheoretic bridge between chemistry and physics.

## 2. Microlevels and Microessentialism

Common metaphysical discussions within the layered picture feature two kinds of ordering structures that overlap: (i) the *mereological*<sup>5</sup> order of whole and part; and (ii) the *metaphysical primacy* order of prior and posterior. In Kim’s words, “the properties of a whole, or the fact that a whole instantiates a certain property may depend on the properties and

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<sup>5</sup> The universe is often conceived as a whole which has its own parts. The investigation of the part-whole relation and its cognates is called mereology. While standard mereology does not tell us what wholes and parts are, it does tell us “what wholes and parts are *given* that other wholes and parts exist”. (Simons 2006: 597 original emphasis)

relations had by its parts. Perhaps even the existence of a whole, say a table, depends on the existence of its parts". (1994: 67) Traditionally, mereological atomism (Atomism for short) tells us that the bottom level in the hierarchy of being is the level of mereological simples or atoms (i.e. objects without proper parts). The atoms are the basic building blocks<sup>6</sup> of the entire world-building. If we conjugate the Hierarchy thesis with Atomism, we obtain the view that "anything of any level except the lowest must possess a decomposition into things belonging to the next lower level"<sup>7</sup> (Oppenheim & Putnam 1991:409). A fundamental property is a property that is not determined by other properties. Whenever entity  $x$  decomposes fully or in part into entity  $y$  or whenever property  $x$  is determined fully or in part by property  $y$ , then  $y$  exists at a lower level than  $x$  (though not the reverse since  $y$  might exist at a lower level than  $x$ , without  $x$  decomposing at all into, or depending at all on,  $y$ .) For example, it is said that oxygen atoms within the  $H_2O$  compound decompose (in part) into electrons, so electrons are at a lower level than oxygen atoms.

The microessentialist thesis according to which we have to resort to microscopic features in order to obtain an adequate characterization of water is often spelled out in terms of "water =  $H_2O$ " or "(all and only) water is  $H_2O$ ". (Needham 2011) The underlying essence of water is its being  $H_2O$ . To use a celebrated Quinean expression, *what*, in the end, *there is*, is to be found on the level of molecules (or whatever the "real" constituents of substances might turn out to be). As van Brakel puts it, to say that "water" is nothing over and above " $H_2O$ " is the same as saying "the essence of water is  $H_2O$ ". (van Brakel 1997:268) In this view, chemical and physical water *really* is  $H_2O$ , and the essence of the transparent substance which we call "water" on the macrolevel and which every human being has to drink in order to survive is, ultimately,  $H_2O$ .

Recently, Needham convincingly argued that the microessentialist claim raises several problems. Typically, the philosophical orthodoxy on

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<sup>6</sup> In Russell's terms, "there are simple things in the universe, and (...) these beings have relations in virtue of which complex beings are composed." (2003:94)

<sup>7</sup> Each level is populated by the entities described by a particular branch of science, and entities at adjacent (proper) levels are related by the part-whole relation, so that every member of level  $i+1$  can be decomposed into members of level  $i$  (for  $i > 1$ ). However, Oppenheim and Putnam also stipulate that any whole that's exhaustively decomposable into parts belonging to level  $i$  also belongs to  $i$ ; thus, the population at each level includes all entities at higher levels. The hierarchy is therefore ontologically conservative in the sense that moving up the ordering does not add any ingredients to the world. All the entities are already contained in the bottom layer, the level described by the most basic theories in physics. (See P. Oppenheim and H. Putnam 1958: 9)

natural kinds relies on Kripke (1980) and Putnam's (1975) writings. Notoriously, chemical substances and biological species are defined as natural kinds. However, while criticism of the application of this line of thought to biological species (Dupré 1981) has already been admitted, criticism of the same line of thought to chemical substances (van Brakel 1986) "has not been similarly acknowledged, and later efforts in the same general direction (van Brakel 2000a and b, Needham 2000 and 2002) seem to have made little impression on philosophers writing on natural kinds". (Needham 2011) As van Brakel pointed out, the underlying microscopic essences vary as much with context or circumstance as the nominal essences: "in liquid water there are  $\text{H}_3\text{O}^+$  and  $(\text{OH})^-$  ions, which are absent in the vapor form of water. On the other hand there are  $\text{H}_4\text{O}_2$ -molecules, as well as other  $\text{H}_2\text{O}$ -polymers in water vapor. And how much there is of each "water-type" depends on the temperature and other contextual variables. The pragmatic answer that water is *predominantly*  $\text{H}_2\text{O}$  is not sufficient if we are looking for essences. A few dissolved  $\text{Na}^+$  and  $(\text{OH})^-$  ions (a drop of sodium hydroxide) don't belong to pure water. Conversely the  $(\text{OH})^-$  ions (of the electrolyte water) that were already there do belong to "normal" liquid water. It is not that we are unsure which (distribution of types of) microstructure is the correct one. The point is that there is not *one* correct microstructure, because the microstructure also depends on the context." (1997: 269-270 original emphasis)

Macroscopic properties afford a characterization of water and classical chemical substances that it not necessary to resort to micro-features for this purpose. As Needham (2011) puts the point, "it is not true, he writes, that we have to turn to microdescriptions for a theoretically grounded, systematic of chemical substances. " Thermodynamics, for example, is a macroscopic theory, traditionally described as neutral with respect to microscopic interpretation) which provides grounds for systematic criteria for characterizing and distinguishing substances. (Needham 2000; 2002)

Although water's microstructure is very complicated<sup>8</sup>, it has already been established that water in the form of ice has a very different microstructure from water in the form of a liquid, and a very different microstructure from water in the gas phase. Contrary to ontological fundamentalism claims, there is no single fundamental microstructure of water. Take the case of *isomerism*<sup>9</sup>. The fact that elemental composition could be common to several substances was first acknowledged in 1820.

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<sup>8</sup> For a detailed treatment of the composition and structure of water see J.L. Finney (2004), "Water ? What's so special about it?" *Philosophical Transactions of the Royal Society of London B*, 359: 1145-1165.

<sup>9</sup> The term "isomerism" was famously coined by Berzelius.

For example, “dimethyl ether and ethyl alcohol, which have the *compositional formula*  $C_2H_6O$  in common, but are represented by two distinct *structural formulas*:  $(CH_3)_2O$  and  $C_2H_5OH$ . These formulas identify different *functional groups*, which govern patterns of chemical reactivity.” (Hendry, Weisberg & Needham 2011, original emphasis)

This leads us to reconsider the view according to which the microstructure of a substance may be somehow independent of macroscopic constraints or somehow determine the macroscopic features of substances in the sense that substances are “nothing but” their constituents. (Needham 2011) The microessentialist might reply that one can appeal to quantum mechanics in order to provide a more unified account of the microstructures. But the case of isomers mentioned above still poses a problem, since, as Needham (2011) pointed out, “the charged particles are precisely the same, so distinct molecular structures are not forthcoming from fundamental quantum mechanics. Molecular properties are in fact calculated on the basis of the Born-Oppenheimer approximation, which in effect imposes molecular structure on the system by taking the atomic nuclei to form a framework around which the electronic motions are calculated. As Woolley puts it, molecular structure “as a universal attribute in molecular science is ... not securely founded in quantum theory” (1978: 1077), but is introduced “by hand” (1988:56) in the course of simplifying and making more tractable the original exact quantum mechanical equations.”

This encourages us to put forward the following working hypothesis: if the microstructures depend on the context in a way that it does not allow us to state which one is *the* one, maybe our current search for *one* fundamental level is deeply misleading. The idea is that [OF] tacitly presupposes a *static* configuration of the ontological layered building hosting fundamental properties.

To sum up, in the previous two sections we have seen that there are serious arguments stemming from recent discussions in philosophy of chemistry against both the view that (i) the higher-level of chemistry is *asymmetrically dependent* on the lower-level of physics, and (ii) that the microstructure of a substance may be somehow *independent* of macroscopic constraints. Consequently, the idea that there will be a complete microphysics that will postulate particles and that these particles are mereological atoms should be rejected. (Schaffer 2003:502) On a closer look, one might realize that the entire layered picture of reality rests upon the hypothesis of a fundamental level added to that of a hierarchical bottom up structure depending on that basic level. But what if both these hypotheses are incorrect? What happens if there is no such fundamental

level, and no sharp distinction between the inhabitants of the levels is possible?

### 3. Priority Monism

Let us suppose that there are no such fundamental simples. After all, it is conceivable that our search for the most fundamental level of reality could, in principle, continue forever. Let us call this hypothesis the Infinite Descent<sup>10</sup> thesis. This possibility cannot be ruled out a priori. As Schaffer puts it, in a boundless world,

it may be true-but-redundant that everything is (in some sense) nothing over and above the subatomic and below, but it will also be true-but-redundant that everything is nothing over and above the chemical and below, and equally true-but-redundant that everything is nothing over and above the psychological and below. (2003:507)

In an infinitely decomposable world, there is no justification for placing a cut-off line between lower level properties and higher level ones. Given that it is clearly unacceptable to merely take some one level as a dependence base (since that would make all properties below that level non-physical), standard physicalism is an “irreparably fundamentalist doctrine.”<sup>11</sup> (Schaffer 2003: 507)

Basically, Priority Monism is the thesis that the cosmos (the whole) is fundamental (i.e. prior to its parts), with metaphysical explanation dangling downward from the One. Schaffer begins by dismissing one common misinterpretation of monism. “Monism is now usually interpreted as the view that exactly one thing exists (van Inwagen 2002: 25; Hoffman and Rosenkrantz 1997: 77). In such a view there are no particles, pebbles, planets, or any other parts to the world. There is only the One.” (Schaffer 2010: 32) But this is misleading, for the central thesis of monism is not that the whole has no parts, but rather that the whole is *prior* to its parts. (Proclus 1987:79)

Without a fundamental level, there is no reason to believe that any infinitely deep dependence base is ontologically more basic than any other. Schaffer gives two main arguments in favor of his Priority Monism:

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<sup>10</sup> “(...) infinite descent yields an egalitarian metaphysics which dignifies and empowers the whole of nature. Treat infinite descent as a working hypothesis, and since all entities turn out to be composite, supervenient, realizes, and governed, it emerges that these attributes cannot be barriers to full citizenship in the republic of being”. (Schaffer 2003:513)

<sup>11</sup> For a position against this view, see Brown & Ladyman 2009.

(a) an empirical argument, based on the idea that current quantum mechanics provides good evidence that the cosmos forms an entangled<sup>12</sup> system; and (b) a modal argument, based on the idea that mereology allows for the possibility of the hypothesis of an atomless gunk<sup>13</sup>, i.e. matter every part of which has proper parts. In what follows, I will leave aside the first argument that has been widely discussed in the literature<sup>14</sup> and I will focus on the mereological argument. If the gunk<sup>15</sup> is possible, Schaffer says, then “heterogeneity all the way down should be possible since such constitutes a consistent distribution of properties over gunk.” (2010:59) The argument from mereology may be phrased as follows:

- P1. Either the ultimate parts must be basic in all worlds, or the ultimate whole must be basic in all worlds.
- P2. There are gunky worlds without ultimate parts (and hence no ultimate parts to be basic in those worlds).
- C. The ultimate whole must be basic in all worlds.

In Schaffer’s view, there are two underlying mereological asymmetries that support this argument.

(a) The first one is *the asymmetry of supervenience*, which states that the proper parts must supervene on their whole, but the whole need not supervene on its proper parts. Differently put, though emergence is

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<sup>12</sup> It was E. Schrödinger who famously coined the term “entanglement”: “When two systems, of which we know the states by their respective representatives, enter into temporary physical interaction due to known forces between them, and when after a time of mutual influence the systems separate again, then they can no longer be described in the same way as before, viz. by endowing each of them with a representative of its own. I would not call that *one* but rather *the* characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought. By the interaction the two representatives [the quantum states] have become entangled. (...) Another way of expressing the peculiar situation is: the best possible knowledge of a *whole* does not necessarily include the best possible knowledge of all its *parts*, even though they may be entirely separate and therefore virtually capable of being ‘best possibly known,’ i.e., of possessing, each of them, a representative of its own. The lack of knowledge is by no means due to the interaction being insufficiently known — at least not in the way that it could possibly be known more completely — it is due to the interaction itself.” (Schrödinger, 1935; p. 555)

<sup>13</sup> For a more detailed discussion on the hypothesis of the atomless gunk see Zimmerman (1996)

<sup>14</sup> See Teller (1986: 71–73); Healey (1991:405–6), Bohm & Hiley (1993: 352)

<sup>15</sup> For an example of a gunky model of classical mereology see Simons (1987:41).

metaphysically possible, *submergence*—the converse of emergence<sup>16</sup>—is metaphysically impossible. For submergence, the intrinsic properties of the proper parts, along with the fundamental relations between these parts, must fail to supervene on the intrinsic properties of the whole. This is impossible because

- (i) any intrinsic property of the proper parts ipso facto correlates to an intrinsic property of the whole, namely, the property of having-a-part-with-such-and-such-intrinsic-property, and (ii) any relations between the parts also correlates with an intrinsic property of the whole, namely, the property of having-parts-thus-and-so-related. Fix the whole, and all of its parts are fixed. (Schaffer 2010:56)

The important idea behind this argument is that the monist can guarantee a complete inventory of basic objects, but the pluralist cannot, for no roster of proper parts can be guaranteed complete, given the possibility of emergence. Schaffer concludes that the whole may well be more than the sum of its parts.

(b) The second underlying mereological asymmetry is *the asymmetry of existence* that stipulates that there must be an ultimate whole, but there need not be ultimate parts. In Schaffer's words, "though atomless gunk is metaphysically possible, *worldless junk*—the converse of gunk, in which everything is a proper part of something—is metaphysically impossible. Classical mereology—with its axiom of unrestricted composition<sup>17</sup>—guarantees the existence of a unique fusion of all concrete objects. Thus there are gunky models of classical mereology, but no junky models. Indeed, a mereologically maximal element is the only individual that classical mereology guarantees in every model. If such models correspond to possibilities, then the only guaranteed existence is the One." (Schaffer 2010: 64) Now, with these new elements in place, let us go back to the layered ontological building. If one wants to reject [OF] and to admit Priority Monism as a plausible thesis, then one has to prove that given our best current scientific theories the Infinite Descent hypothesis is not only an empirically *open* scenario, but also an empirically *supported* scenario. Clearly, quantum mechanics is subject of ongoing investigation. However,

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<sup>16</sup> Entities are said to be "emergent" if they "arise" out of more fundamental entities and yet are "novel" or "irreducible" with respect to them.

<sup>17</sup> The principle of unrestricted composition stipulates that, for any collection of individuals, there is an individual that they compose (with extensionality) as a unique individual, called their mereological sum. Extensionality stipulates that no two things can have the same parts. For a critical discussion of this principle see Simons (2006).

as Schaffer<sup>18</sup> points out, considerations of renormalization in quantum field theory may suggest that “effective quantum field theories might form an infinite tower which “goes down to arbitrary short distances in a kind of infinite regression . . . just a series of layers without end” (Georgi 1989: 456). The crucial thesis here is that if the Infinite Descent hypothesis is true, then there are no simple particles that could suffice to explain everything. We must therefore deduce that there are serious scientific reasons to doubt an ontological picture—Ontological Fundamentalism—which clearly conflicts with one of the most well-confirmed current physical theories, namely quantum mechanics.

## Conclusion

Ontological Fundamentalism is the view that: (a) there is a bottom fundamental level hosting elementary physical particles; (b) all higher levels are ontologically dependent on elementary physical simples; (c) the elementary physical simples are ontologically primary and all the other entities are derivative.

Arguments based on recent developments in chemistry and philosophy of chemistry provide good reasons to conclude, against Ontological Fundamentalism, that: (1) the higher-level of chemistry is not asymmetrically dependent on the lower-level of physics; (2) it is not the case that microdescription will, in principle, always give a more complete description. For example, if quantum mechanics turns out to be wrong, it would not affect *all* chemical knowledge. (van Brakel 1986) The macroworld *is* something over and above the microphysical descriptions underlying it. In light of these considerations I conclude, in line with Schaffer, that Ontological Fundamentalism should be doubted. Priority Monism, i.e. the thesis that the cosmos (the whole) is fundamental (i.e. prior to its parts), with metaphysical explanation dangling downward from the One, provides a more accurate ontological framework for the actual workings of nature.

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<sup>18</sup> Dehmelt (1989) postulates an infinite regression of sub-electron structure. Greene, addressing the question of what strings are made of, allows for two possible answers: “First, strings are truly fundamental—they are ‘atoms’, uncuttable constituents, in the truest sense of the ancient Greeks’. To which he then adds: [H]istory surely has taught us that every time our understanding of the universe deepens, we find yet smaller microconstituents constituting a finer level of matter. And so another possibility (...) is that [strings] are one more layer in the cosmic onion. (Greene 1999: 141–2)” (see Schaffer 2007: 183)



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# CONCLUSION: WHAT HAS PHILOSOPHY TO DO WITH CHEMISTRY?

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Professional chemists, chemical educators, and chemical engineers generally know little about academic philosophy: most philosophers recall only a few scraps of the chemistry they learned at school. Members of both groups tend to use unflattering caricatures as mental images of the practitioners of the other discipline. However, Chemistry and Philosophy do have important common interests. Some of the main long-term problems that chemists face are mainly philosophical: the most-pressing difficulties of contemporary philosophy have substantial chemical components. Philosophy of Chemistry has a great opportunity to do an important intellectual service by bringing these two fields together—and thereby functioning as “*Le Tiers Instruit*” (“The *Learn*-ed Third”)<sup>1</sup> that Michel Serres (1992) described.

The prosperity of ancient Athens that made possible the origin of Philosophy depended in large part on metallurgical chemical technology—which produced substantial quantities of highly valuable silver from the slave-operated lead-mine at nearby Laurion. The roots of Chemistry are even more ancient than those of Philosophy. Yves Coppens (2006) reports that fossils found in a remarkably deep deposit in the Omo Valley in East Africa show that ancient pre-human hominids responded in *two distinct ways* to a slow but severe drying-out that occurred in that area between two and three million years ago. By the end of that long period, *not one but two* successor-species of hominid had replaced the single hominid species (*Australopithecus*) that had prevailed in that location at the beginning of the climatic change. One of these successor hominid species (*Australopithecus robustus*) had followed the same strategy as other sorts

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<sup>1</sup> The first syllable of “Learned” is set in *italics* to suggest that readers use the pronunciation [lɪrˈnɪd] rather than [lɪrnd]. Michel Serres himself uses that (more-antique) English pronunciation.

of animals (elephants, rhinos, pigs, horses, bovids, rodents) and developed large body-size and massive teeth and jaw muscles—suitable for processing tougher arid-area vegetation. In contrast, a second variety of hominid (arguably the first member of the genus *Homo*) had developed a lighter body-form with smaller teeth and larger brain. It is highly probable that the lighter hominids were processing food before eating it—using both physical (pounding) and chemical (cooking) means. Invention of cooking (clearly a chemical process) played a major role in human evolution (Wrangham 2009) long before any pre-philosophical stirrings became important. At the most basic level, what chemists do is to change abundant materials into more-valuable resources—as cooking changes inedible vegetation into nourishing food. Even more than its prehistoric predecessors, contemporary civilization depends—for its flourishing and perhaps even for its survival—on constant improvement of material resources and continual innovation of new ones. A thriving and inventive chemical profession is a *necessary* feature of society—not an optional one.

Chemists face many specific long-term technical challenges—such as how to provide feedstocks for the chemical industry after ancient deposits of hydrocarbons are depleted—but they also must entice bright young people to undertake rigorous education to become competent and creative chemical professionals. They also need to arrange that citizens will become broadly educated—so as to have enough understanding of how nature works that they will support chemical science. These two activities have major properly-philosophical components. Philosophy cannot help solve technical problems in chemical laboratories, but unless chemists and chemistry are widely understood as being important contributors to world culture—and to the “idea of nature” (worldview, *weltanschauung*) of the society—support for chemical work will not long continue. For the survival of their field, chemists must engage philosophical topics more seriously than they have done in the recent past.

Since the ancient Ionian origins of Western speculative thought, discussion of how the characteristics of familiar items depend on their composition and structure has occupied philosophers. Related questions still concern present-day academics. Around the middle of the 20th century a near-consensus prevailed that properties of composites mainly (or solely) depended on the features of components: that “reductionist” opinion is now under serious challenge by other approaches, particularly “structuralism” (Bokulich 2011). The ultimate outcome of these debates is uncertain. Such philosophical discussions frequently invoke chemical terms, but generally at a rudimentary level of scientific understanding. (Some features of current philosophical discourse—particularly those

concerning “possible worlds” or “twin earths”—seem particularly uncongenial to chemists.) But there are many opportunities where effective application of current chemical understanding could contribute importantly to properly philosophic investigation. Nine of the ten items in a randomly-selected recent issue of *Philosophy of Science* can be interpreted as dealing with the major issue of the relative importance of structure and composition in determining characteristics of composites. This is a topic that is closely related to the ordinary preoccupations of chemists—and the understanding that chemists have painstakingly acquired is relevant, but is generally not mentioned in such philosophic debates. Most of the studies in the issue of *Philosophy of Science* selected (October, 2011) pertain to areas of science (particularly Evolutionary Biology) that are, arguably, less well understood than is contemporary Chemistry.

Every chemical investigation can be considered from a variety of philosophical perspectives (methodological, ethical, epistemological, logical, etc.). Contemporary chemistry can yield well-understood examples that pertain to a vast variety of philosophical concerns. In ancient Greek and Latin mythology, Proteus was a sea-god who was capable of appearing in a wide variety of forms. *The Shorter Oxford English Dictionary* defines the adjective “protean” as: “capable of taking or existing in many forms or shapes; changing, varying.” Both Chemistry and Philosophy are immense historically-developed complexes of concepts, behaviors, and practices: each of them is at least as “protean” as is a cloud. On this basis, Philosophy of Chemistry may be considered as the intersection of two moving clouds: a myriad of possible enquiries could properly qualify as Philosophy of Chemistry.

Those brave enough to enter such a field (where others fear to tread) should attend to Whitehead’s caveat: “The mere fusion of all that is would be the nonentity of indefiniteness.” It is essential to *define specific problems that are both amenable to solution and also open up yet further lines of significant research*. Merely filling pages with more or less esoteric jargon should not be accepted. Temptation to combine up-to-date science with obsolescent Philosophy—or current Philosophy with half-understood science—is both common and severe. Adequate work in Philosophy of Chemistry ought to be competent (or better) in relevant aspects of both disciplines. As in other fields, we may expect that greater rewards will come from success in dealing with more-important questions. Deciding which specific problems are worth investigating requires strong background, deep insight, discriminating taste, fertile imagination, and a good bit of luck. As the Editor’s introduction makes clear, all the many contributors to

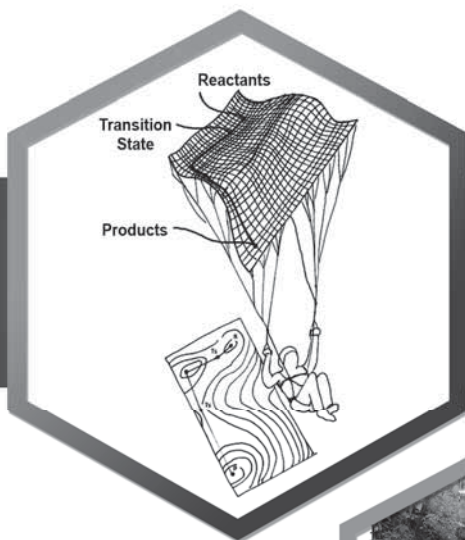


this volume—no matter how different their backgrounds and interests may be—intend to achieve real intellectual progress. But which interactions do in fact bear fruit depends on how we each respond to the work of the others. This not must be a “dialog of the deaf.”

Tertullian, a prolific second-century Christian author, asked “What has Athens to do with Jerusalem?” He concluded that philosophy has little relevance to practical human concerns (and, specifically, it has no importance for the Christian religion). Tertullian’s subsequent life showed that his conclusion was wrong: however, officials in both scientific and civic organizations still endorse the notion that science and philosophy (both terms broadly understood) are mutually independent (e.g., Ayala 2007). But this outlook—like  $P V = n R T$ —has a decidedly limited range of applicability: the more-interesting cases are those in which such simple views do not obtain. Contemporary practitioners of Chemistry and Philosophy need to become better connected, so that both disciplines—and their hybrid offspring—may continue to flourish and to benefit society as a whole. Let us all continue—and extend—the scientific and philosophical integration that this volume achieves.

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## Concepts

### *Part III*



# AFFORDANCES AND HINGES: NEW TOOLS IN THE PHILOSOPHY OF CHEMISTRY

ROM HARRÉ

Traditional metaphysics of chemistry was based on a simple mereology—products of synthetic chemical procedures are the result of the re-arrangement of the constituents of substances that are themselves substances. The results of analytic chemical procedures reveal some of the substantival constituents of the substantival analysanda, those things that are analyzed. As a method in chemical research into the natures of material substances the mereological principle was used in reverse, so to speak. The products of certain chemical manipulations have been assumed to be the constituents of the material substances upon which the relevant manipulations have been practised. I will refer to this as the Product to Part Principle, PPP, and to the associated metaphysical scheme as Daltonian mereology. It has been pervasive in the root ideas of chemistry for half a millennium.

Mulliken's adoption of the expression 'orbital' rather than the Bohrian word 'orbit' shifted the *apparent* ontology of chemistry remarkably little (Mulliken, 1989) However, as Wierzbicka (1997) has argued, the route to understanding a culture, and chemistry is a culture, is via an analysis of the uses of that culture's key words. For the word 'orbit' to make sense there must be 'planetary electrons'-thing-like beings in motion according to the laws of mechanics and electromagnetism. Shifting to 'orbitals' changes the ontological status and hence the meaning of 'electron' in Mulliken's revision of chemical theory. Let us indicate the model objects with the index 'o'. We have 'electron' as an imaginary entity for which we can know only the probability of its location whereas in the original Bohr's theory electrons, presumed real beings, could be assigned definite places. When we read Mulliken's talking of electrons in the context of orbitals, 'electrons' will appear as small 'things', that is as components of the working model, which disciplines the way the Schrödinger equations for each and every electron *are* molecular orbitals. 'The problem of valence,' he remarks (Mulliken, 1989: 89) 'particularly how many and what kind of

atoms can attach themselves to a given atom to form a molecule had long been a central problem of chemistry'. And again: 'In molecular orbital theory, each state of the molecule and of its ions is characterized by an electron configuration giving the number and kinds of MOs [molecular orbitals] and how many electrons are present in each'. Atoms are constituents of molecules and electrons are constituents of both. This is the mereology of the model, not of the world. There is no suggestion that *this* model pictures the world.

However, throughout Mulliken's more public writings on molecular orbitals there runs a notable ambiguity—are orbitals mathematical objects or are they also physically meaningful? The latter interpretation would distinguish MOs as descriptions of supposed real processes and structures from their use to develop working models. In his lecture, (Nobel: 132), Mulliken introduces the notion of 'atomic orbital' as 'an eigen-function of a one-electron Schrodinger equation which is *based on*<sup>1</sup> the attraction of the nucleus for the electron we are considering plus the average repulsion of all the other electrons.' This sounds as if he takes for granted that the equation describes an actual state of affairs. On the next page he introduces 'molecular orbital' in the same way as 'based on the attractions of two or more nuclei plus the average repulsion of the other electrons'. He adds that a true or best MO corresponds to a self-consistent field.

However, it seems from the way he develops his mathematical presentations of molecular orbitals, that the very idea of "atom in molecule" could be read as a reference to a convenient model for managing the mathematics of molecular orbitals as linear functions of the Schrödinger equations for the imaginary binding electrons in each imaginary 'atomic' constituent. This would have been a profoundly radical proposal with important consequences of how we are to understand the metaphysics of chemical manipulations. We seem to be manipulating minute charged material bodies, but 'an orbital is, strictly speaking, just a mathematical function in ordinary 3-dimensional space'. Then follows '... an electron is occupying an orbital ...' a somewhat startling metaphor to follow the previous sentence. Neither in his autobiography nor in his Nobel Lecture does Mulliken come anywhere near resolving the three-way ambiguity. Are molecular orbitals descriptions of the motion of electrons? Are they mathematical devices only? Or are they 'based' on the adoption of the Daltonian mereology as a model? Let us call this the 'Mulliken Enigma'. However, following up the argument so far, the first possibility can be ruled out. In effect Mulliken denied any reality to electrons, though

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<sup>1</sup> My emphasis.

he does not seem to have explicitly identified them with the components of an iconic model.

By way of contrast, in an important discussion of the relation between products and constituents Earley (2005) has used an implicit metaphysical scheme that is built around dispositional concepts. His discussion has been linked to the theory of affordances, dispositions that are created in the interplay between an agent and the possibilities that the target of the agent's activity makes possible. Taking a 'modeler's' attitude to 'atoms' as molecular constituents fits well with the idea that chemists explore the affordances of material stuffs. In the discussion to follow I make an attempt to sketch a schematic layout for a basic metaphysics of chemical science, in the light of this proposal. Let us call this Leibnizean metaphysics. Set aside for the moment are the metaphysical schemes implicit in the discourses and practices of chemical engineers and pharmaceutical chemistry.

### **Traditional Foundations of Chemical Methods**

Methodologically chemical science is built on two basic principles:

The content of chemical knowledge is hierarchical. We share some that the knowledge with Robert Boyle (1667), for example how to prepare Glauber's salt. In Wilfrid Sellars's terminology (Sellars, 1965: 173), taken up by Edwin Hung (2006: 67) we share an external ontology with Boyle but the internal ontology of chemical reactions has changed several times since then. But we can invoke the essentially Dalton mereology of atomic representation of such matters as atomic weights and combining relationships between entities defined according to the elements of the Periodic Table as collections of small bits of stuff. This opens the question of how they held together, a problem discussed by Newton himself in the unpublished *De Natura Acidorum*, written about 1692. Later, probably 1710, it was circulated in manuscript form by Archibald Pitcairne. (Guerrini, 1987) From the beginnings of the idea of valencies as combining powers of atoms, through Davy's and Berzelius' opposite electric charge theory, the next major step was the Lewis electron sharing account of chemical bonding, eventually reaching the deepest level in Mulliken's molecular orbitals. Indeed, Mulliken rejected 'valency' as an intrinsic property of atoms. From the mereological point of view we face the Mulliken Enigma, where it seems we are still today. Our main working model involves substantival concepts, while our best ontological insights reject such concepts as naive.

Theoretical concepts used in creating explanations of chemical phenomena are derived from epoch relative current models of unobservable reality. Transformed and updated versions of Dalton's atoms continue to find a place in the first order explanation of chemical phenomena, for example in the account of the affordance of salt crystals from the evaporation of brine. Second order explanations draw on such Bohr era concepts as the 'noble octet' of shared electrons, and so on. And for third order explanations the shift from orbits to orbitals marks the absorption of quantum mechanics into theoretical chemistry. However, it leaves us with the Mulliken Enigma.

However, the question of the nature of chemical properties as revealed in observation and experiment remains unclear. And that is strange, because that is where we start—smelting iron ore, extracting salicylic acid from willow bark, measuring the percentage of alcohol in a vintage, and so on. A metaphysics based on perceptual categories by attempting to treat chemistry as the science of identifying material stuffs by their colours, shapes and tastes, and chemical manipulations as means for changing them, is unsatisfactory. That was the theory of tropes (Harré 2004). It had a predecessor in the interesting but mostly ignored *The Calculus of Chemical Operations* of Sir Benjamin Brodie (1859).

It also leaves the nature of the chemical properties presupposed in interpreting models or representations of the nature of chemical stuffs and processes that are unobservable in the ordinary way, and even by the microscope, unresolved.

In this discussion, the use of the concept of 'affordance' as the basis of a metaphysics of properties will be explored. I hope that adopting this concept will resolve metaphysical issues at both levels, perceptual and theoretical. However, the affordances of most significance to Mulliken's project were spectra. Without spectroscopes there are no spectra, so we have the format for treating them as affordances. The use of the concept of affordance is made more complicated by the way that chemists have used the principle that chemical analysis of a substance yields products that must have been components of the substance analyzed to reason back from products to constituents, even when the products are affordances. We will spell out these issues in detail below.

## **Textbook Metaphysics**

It is not much good hoping that the metaphysics of chemical science can be left to the chemists. In an otherwise well written and presented textbook R. Chang (2003) offers the following account of properties:

*“Physical properties:* ‘can be measured or observed without changing the composition or identity of a substance’. So we get Dr Chang’s example: ‘Boiling point–boiling changes liquid to gas of the same substance, e.g. Water to steam.’”

*“Chemical properties:* ‘to observe this property we must carry out a chemical change [that is change the composition or identity of the substance]’. Here is his example: ‘Combustibility–burning changes hydrogen gas to liquid, water.’”

This effort begs so many questions it hardly needs philosophical commentary.

## Essences

A distinction between the attributes we ascribe to substances on the basis of common observation and the attributes we cite in explanation of what we observe has been a part of the foundation of physical sciences, particularly chemistry, since the seventeenth century. Locke made famous the distinction between nominal essences, the attributes we use in classifying substances on the basis of observation (semantic category), and real essences, the material constitutions of such substances which they possess independent of observation (a hypothetical empirical category, created through modelling) that accounts for the applicability of the nominal criteria.

In an ideal science there would be a discrete set of criteria for identifying substances by their observable or experimentally displayed attributes and a second discrete set of ‘deep’ properties that would distinguish substances at a fundamental level *and* that the two sets of criteria would match perfectly. This is the principle of the identification of substances in terms of real and nominal essences.

In practice there have been long running dialectical patterns of back and forth revisions in each criterial set driven by empirical and theoretical advances. Essences are context and epoch relative necessities.

But this analysis depends on the assumption that the regresses of chemical knowledge are ontologically homogeneous. Parts of material substances are also material substances. This is the strong meteorological principle, SMP that held sway over chemistry for centuries. Working with the principle that the parts of substances are also substances, and tacitly following Boyle’s recommendations of chemical methods as devoted to breaking up and rearranging clusters of corpuscles, continued to dominate

the metaphysics of chemistry. Mulliken writes as if SMP were true right down to the level of the electrons that 'populate' his orbitals and which are taken to be the material sources of the spectra on which much of the knowledge of the structure of atoms was based. However, as I have argued, this makes sense only as a *confident* usage of a powerful and heuristic model.

### **A Seventeenth Century Way of Interpreting the Relation between Experience and Chemical Structures**

One way of linking observations to the supposed permanent and observation independent characteristics of substances was the concept of 'disposition'. To call something 'red' in the scientific mode was to make a conditional statement of the form 'if seen in a good light the substance will (would, should, might) looks red'.

We are led to say that the word 'red' has a double meaning-'to be red' a substance must have a certain disposition grounded in its real essence, whatever the contemporary theoretical chemists say that is, and 'to be red' a material thing must display a certain sensory quality in a certain kind of situation-defined by apparatus and mode of manipulation. Of course, the link to experience just is the fact that that apparatus is usually the human eye. The 'vocal' or 'inscription' 'red' is polysemic.

The assumption that dispositions and natures were in neat correspondence was indirectly queried by Niels Bohr in particular when it was realised that the physical properties displayed by sub-atomic entities depended on the choice of experimental technique and apparatus, and that these displays could not be comprehended within a single ontological category, discrete or continuous.

The kind of apparatus was an ineliminable part of the apparently descriptive concept seemingly assigning a property to a material entity, e.g. the Bohrian interpretation of the wave/particle dualism. The world in relation to one kind of apparatus displayed particulate phenomena and in relation to another kind of apparatus wave-like phenomena, though the source of each kind of phenomenon was the same. Neither should be assumed to be attributes of the world absent the interaction with the apparatus. We need a new general metaphysical concept to do justice to this turn of affairs-the fact that we seem to be driven to say that the apparatus is not detachable from the phenomena it is supposed to be built to detect or measure. The idea that some products are not constituents already appears in a famous paper by Ambartsumian and Ivanchenko (1930). They propose that certain subatomic particles should be regarded



as products of the experimental manipulations rather than as constituents of the substances from which they are derived.

## Two Necessary Innovations

To do justice to the insight of Mulliken and Earley, both of whom push on the metaphysical limits of post-Daltonian chemistry though in different ways, two basic concepts not currently part of the armoury of philosophy of chemistry need to be introduced. The first is the concept of 'affordance', briefly sketch above, to express a metaphysical innovation essential to understanding the methods and conclusions of chemical research. The second is a development of Wittgenstein's concept of a 'hinge'—an expression he used to refer to the unexamined roots of human thought and action in basic practices and the propositional expressions linked to them.

## Affordances

Already in the mid 20<sup>th</sup> century J. J. Gibson had proposed a general account of perception in terms of affordances—what we know about substances and material situations is what they afford to a human observer in quite definite circumstances. 'The affordances of the environment are what it offers the animal, what it provides or furnishes, either for good or ill. The verb "to afford" is found in the dictionary ... I made up the word "affordance"'. (Gibson, 1979, p.127)

In this paper I develop this idea by generalising Gibson's proposal from animals to human observers to experimental apparatus, in a way that supports Niels Bohr's somewhat opaque philosophy of science and which is of prime importance in the philosophy of chemistry.

According to Gibson, the nature of human perceptual systems and the activities they are used to manage cannot be detached from the perceptual phenomena experienced by human beings. So perception affords experiences—it does not mirror a corresponding material property. 'Affordances cut across the subjective-objective barrier. They are objective in that their existence does not depend on value, meaning or interpretation. Yet they are subjective in that an actor is needed as a frame of reference. By cutting across the subjective-objective barrier, Gibson's affordances introduce the idea of actor-environment mutuality, the actor and the environment make an inseparable pair'. (Mc Grenere and Ho, 2000, p. 2)

There are three root ideas in the Gibsonian concept of affordance:

1. An affordance exists relative to the actual capabilities of a particular actor [and the equipment that is available to him or her].
2. The existence of an affordance is independent of the actor's ability to perceive it.
3. An affordance does not change as the needs and goals of the actor change.

Each of these has an interpretation in the philosophy of physics and chemistry. This is in addition to Gibson's the original interpretation of affordances as features of human perception of interest to psychologists.

Niels Bohr's philosophy of physics is notoriously difficult to interpret in the concepts available to us from traditional philosophy of science. Applying the notion of 'affordance' to the task of Bohrian interpretation we reach the following insight: the apparatus, its nature and way of working cannot be detached from physical phenomena (observations). An electron producing apparatus does not display particulate constituents of the atoms from which they seem to come-but affords subatomic particles to the experimenter using the apparatus in a certain way. With a different apparatus the experimenter can get the world to afford interference phenomena with the same starting point as the experiment that afforded particles. It is a mistake to read back from product to constituents—atoms do not contain electrons as components, but they are such as to afford electrons to a suitable apparatus and manipulations.

In a similar way, but seemingly more radically, we could say that experimentation affords chemical phenomena in the appearance in solutions of such entities as ions—from which it does not follow without some further principle that ions are constituents of molecules. As we follow Mulliken's development of molecular orbitals through the shift of nomenclature from orbit which a thing-like being might occupy to an 'orbital' which in a sense is 'occupied' but only by semantic courtesy of the abandoned concept of 'orbit'. Moreover, throughout Mulliken's writings spectra as affordances play an important role.

A Davy apparatus does not display a congealed mass of metallic constituents of salts, but affords a sample of sodium metal. That a block of sodium metal safely immersed in paraffin is made of constituents of common salt requires an additional metaphysical principle that may turn out to be hard to find.

## Hinges and Hinge Propositions

Querying the universality of the principle that it is rational to infer the nature of the constituents of a substance from the nature of the products of action directed to 'disintegrating' that substance, leads into some deep philosophical waters. I will argue that the Product to Parts principle is a hinge, in the sense of later developments of Wittgenstein's use of the expression in *On Certainty* (Wittgenstein, 1979). In many contexts it provides the missing principle referred to in the previous section.

Developments of this idea by Moyall-Sharrock (2004) and others has led to the identification of hinge practices, activities we perform without taking account of their presuppositions, such as reflecting on what happened yesterday, going into the men's room without even considering the possibility of taking the adjourning door and so on. These practices remain firm while all sorts of other practices can change, for example asking one's companions what happened yesterday, looking at a diary entry and so on. The character of these practices is revealed by reflecting on the logical status of the propositions that seem to go along with them—their doppelgangers, as Moyal-Sharrock calls them. In the case of reflection on yesterday's events, a suitable doppelganger would be 'There have been events before those now occurring'. This proposition is the doppelganger of a hinge practice fundamental to human life. It might look as if it is a necessary truth. For example, the very concept of 'the present' makes sense only if the concept of 'the past' makes sense. But reflection suggests that it is a very general empirical proposition that could have been false. The meaning of 'is past' might be linked to that of 'is present' but it does not follow that there must be something to realize that concept. The meaning of 'ghost' is linked to that of 'dead person' but it does not follow that there are any ghosts. The same holds for Wittgenstein's examples of 'I am a man' and 'No one has ever been on the moon'. Fraulein Ludmilla Wittgenstein is a possible person and people have been on the moon.

In short, a hinge practice shapes a form of life and its doppelganger, a hinge proposition is an empirical proposition that is not generally called to mind and rarely queried. Though a hinge proposition seems to have some of the features of a necessary truth nevertheless it is possible that it could be false.

I will argue that PPP, the principle that would license projection of the products of a chemical procedure on a material substance back on to that substance as its constituents is a hinge practice and its doppelganger, true for some types of chemical reaction, is not true for others. This opens up the possibility that there are some affordances, such as line spectra, to

which PPP does not apply. And perhaps this opening extends to electrons as constituents of atoms and even to atoms as supposed constituents of molecules.

## Metaphysics of Classical Chemistry

Since the 17<sup>th</sup> century, chemistry has been based on the mereological principle—that the **products** of certain chemical manipulations (to be called analyses) are constituents or **parts** of the substance(s) from which they were derived. Other substance changes are the result of exchanges and rearrangement of constituents.

Varieties of the mereological principle have arisen in discussions of just what constituents are supposed to be—for example the long running atomic theory of material molecules. [See Needham (2005) and Earley (2003) for a discussion of the refinements needed to adjust mereological principles to chemical knowledge.] Even within the refinements introduced by the Needham/Earley debate we must query the simplistic epistemological/metaphysical thesis of a one to one correspondence between observable attributes and permanent material properties of the substances we observe and manipulate.

*How* do we get from products of experimental manipulations to constituents of material substances? This question is made more problematic by the fact that chemical research—driven by theories of chemical bonding—forces us to cross the boundary from a homogeneous to a heterogeneous regress, about which more below,

Turning now to the Product to Part Principle—PPP—it seems clear that it is the doppelganger of a cluster of hinge practices, such as analyzing a chemical compound by subjecting it to certain manipulations that yield products different from the original substance, and that could not have come from a source external to the closed system of the experiment. However when we reflect on the status of the doppelganger proposition—that the products of a chemical analysis are constituents of the analyzed substance, it is clear that this proposition, though sometimes true, is conceivably false.

Electrons figure as the ontological roots of the Lewis theory of chemical bonds. However, as 'constituents' of atoms they do not meet the requirements for the identity criteria of things. The notion of 'an electron' as a numerically distinct being would require that there should be some way of labelling *one* electron in such a way as to distinguish it from all others. No such way has been found or even imagined. Yet electrons as products in certain circumstances follow distinct spatio-temporal trajectories.

## Homogeneous and Heterogeneous Regresses

This distinction is taken from Stroll's (1994), interpretation of Wittgenstein's treatment of psychological and neurological concepts. The most important systems of knowledge are hierarchical, stacks of layers or levels. These are regresses in that they are related layer to layer in various ways, including part-whole, so that in the physical sciences their constituents usually differ in scale.

*Homogeneous Regress*: at each level the metaphysical status of the basic entities remains the same—material substances, for example, are the constituents of material mixtures.

*Heterogeneous Regress*: at some point the next level in the analysis imports entities of a different metaphysical status. For the explanation of chemical bonding, material substances yield to electromagnetic fields.

Physics as an integral part of some larger conception of chemistry seems to involve a shift from a homogeneous regress to a heterogeneous regress. The Lewis 'entities' are electromagnetic, and cannot be treated as individual material substances. However, at the foot of the initial homogeneous regress we seem to have molecules [the role of atoms is another issue] and they are individual material substances with criteria of identity based on continuous space-time trajectories and preservation of relevant material properties.

Crossing the boundary between the two homogeneous parts of a heterogeneous regress forces a change in the ontology of the science or other theoretical enterprise where it occurs. If such a break occurs in the underpinnings of chemistry so a revision of the metaphysics of the PPP product—constituent relation is one of the responses that a philosopher might make to clarify the situation.

## Metaphysical Basis of Chemically Relevant Physics

Atoms were structures of enduring parts that could be extracted as individuals, atoms, ions and so on. Lewis electron theory of chemical bonding introduced a mereological puzzle in the chemically relevant heterogeneous hierarchy of material part/ whole hierarchies. In what sense are electrons *parts* of atoms?

Clearly electrons 'within' atoms are not things—problems about criteria of identity of electrons as constituents of atoms, which are things with respect to criteria of material identity, for example enduring and traversing continuous trajectories. We can turn to Bohrian developments in physics—Bohr resisted the idea that the products of subatomic experiments were

constituents of the material from which they had come.

## **Powers and Liabilities**

There is another distinction from folk chemistry that plays a role in chemical research practices.

1. Chemists have routinely distinguished active substances from inactive in experimental manipulations to determine the best interventionist strategies in an experimental program.
2. Berzelius' binary molecular structure scheme required two electrically active components mutually attracting one another.

Some substances are treated as agents and some as patients—and this distinction is repeated at each level of the mereological hierarchy. Simple experimental chemistry assigns causal powers to some substances, such as acids and alkalis, and not to others such as metallic ores.

- a. Electron donor and electron receiver (Lewis) theory of molecular coherence shifts the locus of activity or causal power from the observable/manipulable level to the level of constituents.
- b. Thus we have the familiar powers/nature regress. Acidity is a power expressed in chemical phenomena, accounted for by the constitution (nature) of the active substance—that is, it is an electron donor.

Redox reactions reinstate the power/liability distinction in terms of electron donor/electron receiver distinction.

However, here we have the Daltonian mereology in up-dated guise, and with a realist intention despite the background presence of the Mulliken Enigma.

## **Is this a Sketch of a Deep Metaphysics of Chemistry?**

### **Modality**

Needham and Earley make the point that the mereology of chemistry must have a modal dimension. Relative to the results of experiment and observation the attributions of chemical properties to substances must be expressed as possibilities. So the form of the attribution of properties to substances must be conditional, that as dispositions.

However, such attributions are, as I have argued, affordances. That is, explicitly or implicitly they are loaded with the presumption of a method and an apparatus, usually a type of equipment necessary for the property to be displayed. Even the sodium and chlorine, existing as ions that survive Earley's examination of the salty affordances of brine are also affordances.

Let us use the word 'instrumentarium' to refer to the range of experimental equipment that is available to scientists in the storeroom of the laboratory in which he or she works and in the catalogues from which (if there is enough money available) more equipment can be purchased. Note that not so long ago the efficacy of an experimenter depended on his or her own skill in the construction of apparatus to add to the local instrumentarium.

Adopting the affordances metaphysics requires the specification of two possibility domains.

- A. The domain of possible set-ups–apparatus/world complexes. [I could not complete my childhood project of isolating the halogens because there was no glass apparatus that would contain fluorine.]
- B. The domain of possible displays brought about by using a possible apparatus-world complex.

However, unlike folk chemistry, the metaphysics of chemical science can do no more than make use of invented models for the indeterminate attributes or real essences of the material substances experimented upon. That is trans-experimental attributes ascribed to chemical substances are conceptual not empirical possibilities.

We cannot detach the causal powers of the world from the world/apparatus in which they are displayed epistemologically. How they are manifested depends on the system with which we interact with the world—our own perceptual devices, such as eyes and ears or the complex and ever-developing apparatus that chemists and physicists create to elicit the affordances of the world in more and more closely defined situations. Commonsense is pushing us in the wrong direction in this matter—the metaphysics of fishing for example. The sea *affords* different species of fish to fishermen depending on the equipment they are using to catch them—line and hook, net, lobster pot and so on. But the fish were there in the sea before they were caught. Electrons were not *there* in the hot wire before they were extracted by a magnetic field.

### The Fundamental Questions

1. What does the instrumentarium afford to a knowledgeable chemist for the construction of world/apparatus complexes?
2. What does such a world/apparatus complex once constructed afford to a skilled experimentalist?

Perhaps we can give these questions content by thinking of Humphrey Davy and his very large battery with which molten common salt was

shown to afford a lively metal.

Running the apparently common-sense principle that products of disintegration must be constituents backwards, we have a route to the construction of plausible *models* of the constitution of material substances. Once we realise that the need to interpret chemistry in terms of affordances forbids us to make claims about the constituents of substances on the basis of the nature of the products of their disintegration we can see that the only possibility for an atomic metaphysics of chemistry is as the basis of innumerable and extremely valuable models.

## Summary

Chemical metaphysics has been Lockean, based on a historical dialectic of nominal and real essences, for several centuries, and for the most part chemists still use Lockean metaphysics as a hinge, with the Daltonian mereology as a picture for establishing the details of the models in use in Lockean chemistry. The dual essences are linked by the concept of 'disposition'. This can be refined as 'affordance'. Affordances are displays produced by specific manipulations of actual locally constructed apparatus. Some of these displays consist of material stuffs. The Lockean scheme calls for them to be grounded in real essence hypotheses. Of what do real essences consist?

Traditional metaphysics of chemistry was based on simple substantialist mereology—products are constituents of substances. I have labelled that principle PPP. In examining PPP there seem to be three interpretational options that we should consider.

1. Products are constituents of the substance from which they were extracted. This is the common hinge on which most of our chemical practices turn.
2. Products can be used via an analogue of PPP to serve as the basis for models of the structure of the substance that was their 'source'. This is a more sophisticated hinge on which some of our scientific thinking turns.
3. Products are affordances, that is cannot be described independently of the devices and methods used to reveal them—and are not constituents of the substance which afforded them to such and such a manipulation. This is a hinge on which the most sophisticated scientific thinking turns.

Doubts about the first interpretation have been raised by Earley's discussion of the apparently paradoxical proposition—'there is no salt in the sea'. Perhaps the fact that chemistry seems to demand heterogeneous



foundations in electromagnetic 'entities' if we base our picture of matter on the idea of constituents bound together by 'something' to create robust aggregates,

In the most successful theory of chemical bonding, Mulliken's 'molecular orbital' or MO theory, the status of the constituents of molecules is not clear, or perhaps we might say, it cannot be made clear. Are Mulliken's 'atoms' by reference to which he distinguishes the component Schrödinger equations of his molecular orbitals, items in a working model? Or, are they occupants of space and time in something like the way molecules are occupants of space and time? This is the Mulliken Enigma. However, if we adopt the concept of 'affordance' to resolve it we are faced with a profound rethinking of the metaphysical basis of chemical science.

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# THREE CONCEPTS OF CHEMICAL CLOSURE AND THEIR EPISTEMOLOGICAL SIGNIFICANCE<sup>1</sup>

JOSEPH E. EARLEY, SR.

## Substrates and Bundles

At least<sup>2</sup> since David Hume rejected John Locke's supposition that properties *inhere* in "substrates" and argued instead that objects are nothing but "bundles of properties," philosophers (mainly English-speaking) have debated how properties hold together in ordinary objects. Currently, Locke's substrate theory has vigorous proponents (e.g., Sider 2006) but a larger number of philosophers favor versions of Hume's "bundle" approach and assert that a "compresence relationship" holds properties (or "tropes"—individual instances of properties) together (e.g., Robb 2005, Simons 1994). When intelligent people carry on vigorous debates about important matters for extended periods, it sometimes turns out that all parties to the dispute have made unwarranted assumptions, or that both sides have overlooked important considerations. This paper suggests *that time cannot be ignored in discussions of properties* and that *coherence of the properties of each individual entity requires closure of networks of relationships between and among components*. Such closure is an important aspect but has not been considered in substrate/bundle debates.

Jiri Benovsky (2008) examined more than six current versions of both substrate and bundle theories. Some of those versions involved "tropes" and others recognized "universals," some had a single identical unification-relation for all objects, others had a single unification-relationship but allowed variable numbers of relata ("polyadicity"), still others had distinct unification-relations for each object. Benovsky

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<sup>1</sup> An earlier version of this paper was presented on September 11, 2010 at the workshop "Epistemology of Chemistry: roots, methods and concepts" held at the *Centre de Recherche en Épistémologie Appliquée, École Polytechnique*, Paris, France.

<sup>2</sup> This debate is related to controversies in ancient philosophy. (Earley 2009)

considered, in some detail, how proponents of each of these approaches defended themselves against objections. At the end of this inquiry, he concluded that both substrate and bundle theories *share* a common central postulate: namely, that each object has a feature, different from all other features of the object, which functions as a unifying device. (This unique feature is called the “substrate” or “bare particular” in one theory, and designated the “compresence relationship” in the other approach.) Benovsky identified both of these postulated special features as *theoretical entities* (items that are “individuated by their theoretical role”) and pointed out that both “play the same role in the same way” in all their applications—therefore the two special features should be regarded “as identical (*metaphysically equivalent*)” (p. 183). Benovsky concluded that substrate and bundle theories are “twin brothers” rather than “enemies”—and that both these approaches are seriously deficient, since neither has succeeded in clarifying the nature of the basis of unification that they both require.<sup>3</sup>

### Property Persistence through Interaction

Remarkably, recent participants in substrate/bundle discussions seldom or never mention findings of physical chemists regarding how properties of well-defined chemical substances relate to the composition of those materials. Hilary Putnam (1969) pointed out that philosophers often encounter serious problems because they generally use the word “property” to denote *anything that can be said about an object—any “predicable.”*

Philosophers who discuss substrate and bundle theories seem mainly concerned with *logical* structure, proper modes of speech, and maintaining customary patterns of thought (respectfully designated as “intuition”). Chemists have different priorities<sup>4</sup> and generally use a more-restricted

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<sup>3</sup> Mathematicians recommend that if a particular problem proves to be intractable then one should make a strategic switch to a different and easier problem that retains important features of the original task (Polya 1985). If the second problem can be solved, that solution may provide tools or hints that will allow the original problem to be clarified. The objects discussed in substrate or bundle debates have generally been ordinary items encountered in everyday life—e.g. roses, tennis-balls, statues. Perhaps, as the mathematicians suggest, greater success might be obtained by considering items that are less familiar but are understood in more detail, such as the entities with which contemporary chemists deal.

<sup>4</sup> It seems that participants in these debates have little concern as to whether the features they postulate are in fact exemplified in nature. In Shakespeare’s *King Henry IV, Part I*, Welsh chieftain Owen Glendower boasts: “I can call spirits from the vasty deep.” His English cousin and rival Hotspur replies: “Why, so can I, or so

concept of property—one described by American chemist and philosopher Charles S. Peirce [1839-1914], who defined a property as *how a thing behaves, or would behave, in a specified operation*. This usage exemplifies Peirce's "pragmatic principle" (1878).

Consider what effects, that might conceivably have practical bearings, we conceive the object of our conception to have. Then our conception of these effects is the whole of our conception of the object.

All the entities with which chemists deal are somehow composed of smaller items. All of these objects (both composites and components) are known to be in incessant thermal motion and also in continual interaction with other items. In order for any composite to remain more or less the same through motion and interaction there must be features of that composite that insure sufficient resiliency for integrity to be maintained. Paul Weiss (1959) described this situation well:

Each actuality is a substance. It maintains a hold on whatever it contains, produces, and intrudes upon. It persists and it acts. It has an irreducible, independent core, and receives determinations from insistent, intrusive forces. ... If an actuality were not a substance, its parts would not belong to it, and it would disperse itself in the very act of making its presence evident. The very items which it dominates, it would not control; nor would it continue to be despite an involvement in change and motion. It would be inert and solely in itself, or it would be a mere event. In either case, it would not be a source of action.

The well-established dynamic aspect of nature—incessant motions of all items—requires an account of the factors to which Weiss calls attention: how properties of objects are maintained through time, how they interact with others, and how they maintain their own integrity during such interaction.

Participants in substrate/bundle debates generally ignore temporality and explicitly or implicitly adopt "synchronic" approaches in preference to "diachronic" ones. (Humphreys 2008, Earley 2003b) The shared (but certainly false) assumption that history is negligible seems to have been a major factor contributing to the failure of both conceptual schemes (Earley 2012). The long-term stability of composite chemical entities—molecules of dihydrogen or crystals of table salt for instance—even while the

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can any man; But will they come when you do call for them?" (Act 3, Scene 1.) Hotspur probably would approve chemists' use of Peirce's pragmatic concept of properties.

components are in constant motion requires that such motion is somehow *constrained* so that the entities maintain their integrity. We now consider how such coherence is achieved.

### Closure Louis de Broglie

When Louis de Broglie resumed his study of physics after the close of World War I, the then-existing theories of Bohr and Sommerfeld could adequately rationalize the extensive body of experimental data that was available on the line spectra of atomic hydrogen and ionized helium—but only by making the unsupported assumption that electrons in atoms are restricted to certain specific energy values (“orbits”). As de Broglie pointed out in his 1929 Nobel Prize address, those early versions of quantum mechanics *could not* explain: “why, among the infinity of motions which an electron ought to be able to have in the atom according to classical concepts, only certain ones were possible.” In a note in *Comptes rendus*, de Broglie (1923) proposed that each electron within an atom had a frequency intrinsically associated with it, and also was connected with a wave that carried no energy.<sup>5</sup> He then introduced a postulate:

It is almost necessary to suppose that the trajectory of the electron will be stable only if the fictitious wave passing O' catches up with the electron in phase with it: the wave of frequency  $\nu$  and speed  $c/\beta$  has to be in resonance over the length of the trajectory.

This postulate envisions that an atomic system will be stable (that is, will persist) only if two oscillations agree in phase. The “only” in this postulate (emphasized in the French original) is a clearly a requirement of a specific relationship between two quantities (phases of waves). On the basis of this postulate, de Broglie was able to derive the Bohr-Sommerfeld criteria for stable states of the electron in the hydrogen atom. This was a great triumph: de Broglie was awarded the 1929 Nobel Prize for Physics on the basis of his 1924 doctoral thesis.<sup>6</sup> The essential novelty of this

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<sup>5</sup> Later, this “fictitious wave” became known as “the phase wave” or “the pilot wave.”

<sup>6</sup> Through Einstein’s mediation, this thesis also inspired Schrödinger’s development of wave mechanics. In the contentious Solvay Conference of 1927, de Broglie’s approach was criticized by Wolfgang Pauli and others, and was then largely supplanted by Bohr’s “Copenhagen Interpretation.” (Bonk 1994) Recently, de Broglie’s approach has been partially revived by Bell, and used in models of the internal constitution of the electron.

contribution was that it provided *a criterion* that served as a basis for understanding *why* some states of electrons in atoms were capable of extended existence while other apparently equivalent “states” were not capable of existence.

Related sorts of closure and analogous criteria are, I submit, characteristic of *all* stable chemical entities. The general requirement for such criteria is a key factor that has been left out of past and current philosophical discussion of bundle and substrate theories.

## Molecular Properties

In chemical entities, distances between components remain within narrow limits because of *balance of attractive and repulsive interactions* (a type of closure). Attractive forces tend to pull components inward while repulsive interactions impel those constituents outward. As the positive centers separate for whatever reason, attractive forces draw them back together. Figure 1 (below) displays calculated curves showing how potential energy varies with distance between positive centers for the three lowest-lying electronic states of the dihydrogen molecule,  $H_2$ . The upper and lower curves correspond to situations in which the two electrons have opposite spins (“singlet states”). The central curve corresponds to a circumstance in which the two electrons have the same spin (a “triplet state”). The lowest curve features a minimum which corresponds to a potential energy that is more negative (lower) than that of the uncombined atoms. The central curve has no minimum. The third curve has a minimum but at a value of potential energy that is less negative than that of the free unexcited atoms, and at larger internuclear distance than corresponds to the minimum in the lower curve.

If two hydrogen atoms with opposite electronic spins were to collide and somehow to transfer energy to a third body (say, a helium atom or the wall of a reaction-chamber) a dihydrogen molecule might result. Once produced, this two-centered entity would move through space as a unit—while vibrating more or less vigorously (that is, as it oscillates within the “potential-well” defined by the minimum in the lower curve in Figure 1) (Earley 2003a). Texts in physical chemistry and quantum chemistry show that factors that determine the potential-energy versus distance curves for dihydrogen are now rather well understood.

### Three Concepts of Chemical Closure

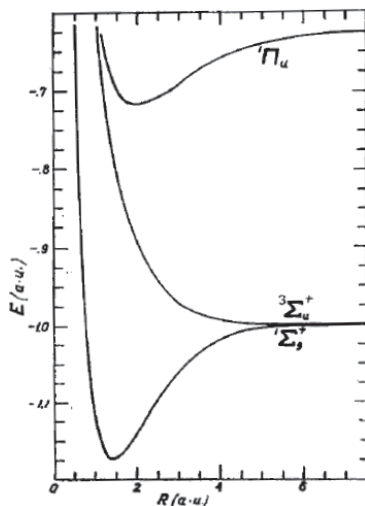


Figure 1. Calculated potential-energy curves for the dihydrogen molecule. (Taken, with permission, from Kolos 1965)

Properties that depend only on the constitution of dihydrogen molecules could be interpreted as deriving directly from the potential-energy versus internuclear-distance curve. The molecular weight would be one such property.<sup>7</sup> Two other types of properties are of great interest to chemists.

*Spectroscopic* properties involve transition between various stable energy states of a given molecule with concomitant emission or absorption of energy. *Chemical* properties involve interactions (of molecules with like or different others) that lead to transition to a different potential-well corresponding to alternative molecular compositions, or to new arrangements of connection of elemental centers.

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<sup>7</sup> If a nonvolatile molecular substance were introduced into some appropriate volatile solvent, the freezing and boiling points of that solution would differ from the corresponding values for the pure solvent. For a dilute solution, both the boiling-point elevation and the freezing-point depression would be proportional to the lowering of vapor pressure of the volatile solvent due to presence of the nonvolatile solute. Such "colligative" properties of solutions depend on the number of molecules of a given type that exists in a specific volume of solution and are not influenced by the properties of individual solute molecules. This would be another strictly "molecular" property.



## Spectroscopic and Chemical Properties

Vibrational and rotational energies are “quantized”—restricted to specific values that are spaced in regular ways—just as electronic energies are. Energy levels are spaced more widely for electronic states, less widely for vibrational states, and quite closely for rotational states. Figure 2 (below) shows the several vibrational states that correspond to the two low-lying electronic states of the dihydrogen molecule that have potential minima. Each of these vibrational states has several associated rotational states. The designation ‘state’ implies that, absent any disturbance, the system might remain in any one of these conditions indefinitely.<sup>8</sup> But transitions between states can occur: such transitions provide the means for the molecule to interact with the rest of the world while retaining its integrity as dihydrogen, by maintaining the H—H bond. *Closure* is what allows each molecule to “make a difference” (Earley 2008, 2006; Ney 2009).<sup>9</sup>

Detailed study of “spectroscopy”, the energy absorbed or released when chemical systems change for one energy state to another, accounts for much of the success modern chemical science. For a single instance, Martini et al (1990) used emission from the first vibrational excited state of dihydrogen to the ground (lowest) state to gather information about conditions in several “reflection nebula”—immensely distant galaxy-clusters that are thought to be regions of active star-formation. Consideration

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<sup>8</sup> For this reason the middle curve in Figure 1 does not correspond, properly speaking, to a state. The “triplet state” designation is used “by courtesy.”

<sup>9</sup> Transition from a state associated with the lower electronic curve in Figure 2 to a state associated with the upper curve would involve a dihydrogen molecule absorbing a photon of appropriate energy. Once in the upper well (with a longer distance between the elemental centers) vibrations and rotation could occur. Sooner or later the molecule would emit a photon and move to one of the states associated the lower curve, or the molecule would split up into free atoms. Transitions between molecular energy states are subject to a restriction chemists call “the Franck-Condon principle”: *no nuclear motions occur during state-to-state transitions*. Notice that in the figure lines indicating transitions are all vertical. This restriction applies because nuclei are relatively heavy and therefore move vastly more slowly than nearly weightless electrons. In this consideration the parts of the dihydrogen molecule are taken as two protons and two electrons of opposite spin. Even though the formula of dihydrogen is H<sub>2</sub>, that molecule does not “consist of” two hydrogen atoms. Strictly speaking there are *no* atoms “contained in” dihydrogen or any other molecule. (It appears that most philosophers are misinformed on this elementary chemical concept.)

of the details of the closure of relationships in the dihydrogen molecule is essential to account for the observed colors of these nebulae.

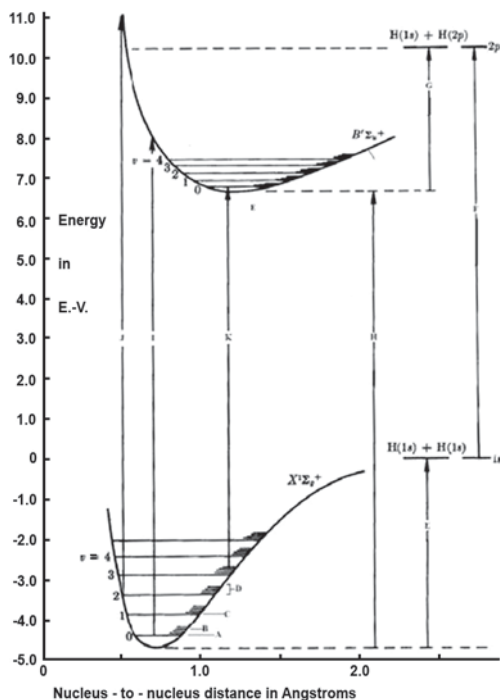


Figure 2. Electronic, vibrational, and rotational energy levels for the dihydrogen molecule. (After Kolos 1965, with permission.)

Stability of any chemical species corresponds to a closure of relationships that defines a minimum of potential energy for a specific pattern of connectivity of elemental centers. The details of each such potential-well determine how each composite entity interacts with other systems, and so specifies the properties (in Pierce's pragmatic sense) of that coherent unit.

The central and essential parts of chemistry have to do with turning less-valuable materials into more-valuable items—making cheap stuff into expensive stuff. Chemical reaction corresponds to transition between stable states—change from one potential-well to another. Chemical reactions correspond to production of *new closures*—every chemical process is “*a becoming*.” (Earley 1998b) Every chemical change involves decrease in

“chemical potential” (free energy) but transition from reactant to product potential-wells necessarily involves passage through intermediate configurations that correspond to higher potential energy. Slow rates of chemical reaction involve traversing configurations that correspond to such “barriers” of higher potential energy between reactant and product configurations.<sup>10</sup>

### Closure Henri Poincaré

Discussions of composite objects generally assume (implicitly or explicitly) that properties of composites depend only (“supervene”) on the properties of components. That is, the properties of the lowest (“ultimate mereological”) level determine all properties (e.g. Armstrong 2010, pp. 29 ff.). Characteristics of dilute gases can sometimes be inferred from information regarding component molecules—based on the approximation that each molecule acts fully independently. However, when gases are cooled so that conditions come closer to those of the gas-liquid transition, correlations of molecular motion develop—first over short ranges, then over longer and longer distances. The result is that motions of individual molecules are no longer independent but rather become more or less interrelated.

Similarly, the simple model that chemical reactions occur by “elementary steps” that all involve “instantaneous” collisions of pairs of molecules is usually an oversimplification. Frequently, “sticky collisions” produce “resonances”—more or less persistent aggregates. These also give rise to correlations among molecules. For an example of resonances in a simple reaction, the reaction between a beam of F atoms and a second beam of HD molecules shows non-linearities in the energy versus reaction-rate (“cross-section”) profile that are interpreted as arising from the presence of three rotational states of a tri-nuclear resonance transiently formed in this exceedingly simple reaction (Dong 2010, Althorpe 2010).

In both phase-change and chemical-reaction cases, as correlation increases applications of “fundamental” theory become unwieldy and impracticable. In fact, under certain conditions (at “singularities”)

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<sup>10</sup> For instance, change from the stable *cis*-conformation of 1,2 dichloroethane to the equally stable *trans* -configuration encounters only a small barrier: the corresponding reactions of 1,2 dichloroethylene encounter a larger potential-energy barrier and hence are much slower. Properties such as the melting temperature of a solid or the boiling temperature of a liquid could be considered as chemical properties, referring to especially simple chemical reactions involving interaction of molecules of only a single type.

theoretical computations turn out to be *impossible in principle*—as computed quantities rapidly go to infinity. In the late nineteenth century, while investigating the motions of the planets, Henri Poincaré encountered situations in which standard methods failed due to the occurrence of singularities. In such cases, in regions near the singularities, he replaced the usual variables with divergent series (“asymptotic expansions”). This technique (Berry 1994) often led to discontinuous change (at the singularities) in the equations that described the dynamic situation. At and beyond each singularity, Poincaré found that relatively simple expressions applied: these new equations generally emphasized contextually important features and suppressed irrelevant detail.

When use of such asymptotic expansions becomes necessary for chemical calculations, plots of “reduced” (unit-less) variables typically show lack of dependence on properties of individual substances. For instance,<sup>11</sup> at various *reduced temperatures* ( $T/T_c$ ), compression factors of many gases *have the same* dependence on reduced pressure ( $P/P_c$ ) independent of their quite diverse individual properties. (Moran 1995) That is to say, properties other than those that influence critical behavior are *effectively irrelevant* to deviations of gases from ideal-gas behavior.

The simpler description that asymptotic expansion yields at and after singularities has different semantics (another “topology”) than the “fundamental-level” description that applied before the singularity. Properties of highly correlated systems do not “supervene on” properties of components of the system but require quite new (and topologically incommensurable) descriptions (Batterman 2009, 2005, 2002, 1998; Bishop 2006, 2005; Primas 1998, 2000). A Nobel laureate in Physics has argued (Laughlin 2005) that many aspects of “fundamental” physics *result from* such cooperative interactions.

Cooperative interactions in condensed phases sometimes yield spectacular results. For instance, at room temperature, cesium chloride crystals can exist in two different spatial arrangements—one with six positive ions around each negative ion and one with eight. One structure is more stable at lower temperatures the other form is more stable at higher temperatures—but conversion between the two structures does not occur rapidly. At a particular temperature a given crystal of this salt might have either internal structure, depending on its prior history. Transition from the unstable to the stable form of cesium chloride does not occur smoothly and gradually, but rather happens abruptly—usually with an audible click that

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<sup>11</sup> At “the critical point” [critical temperature,  $T_c$ ; critical pressure,  $P_c$ ] distinction between liquid and gas phase disappears. Compression factor,  $Z = P V_m / R T$ , measures deviation from ideal-gas behavior. ( $V_m$  = molar volume.)

is accompanied by fragmentation of the crystal. This remarkable behavior (a *Martinsitic* transition) is interpreted as occurring by coordinated and simultaneous small motions of immense numbers of ionic centers (Chakabarti 1979, Earley 2003c).

When cooperative interaction of units becomes dominant, situations adequately described by fundamental theories change into to situations that require approaches that use quite different sets of entities and relationships (other “topologies”). This type of transition is also a kind of closure—a type of interaction that brings about epistemological and ontological change. (Primas 1998) We call this circumstance “*Closure Henri Poincaré*.” Occurrence of such closure vitiates assumptions that properties of chemical entities can be adequately understood on the basis of descriptions based on properties of component parts, as Humean presuppositions imply. This situation was well described by Hans Primas.<sup>12</sup>

The task of higher level theory is not to approximate the fundamental theory but to represent new patterns of reality... According to quantum theory the material world is a whole, a whole which is not made of independently existing parts. ... Quarks, photons, electrons, atoms or molecules are...contextual objects without an independent existence. (Primas 1998)

### Closure Jacques Cauvin

Investigation of the properties of networks of processes (such as interconnected chemical reactions) is one of the most active fields of twenty-first century science. Surprisingly, in some biological situations, critical reagents involved in networks of reactions somehow remain at quite constant concentrations for long periods. A remarkable theorem as to how this can come about was published in Spring 2010 (Shinar and Feinberg 2010). To understand this achievement, we need some concepts that are illustrated with reference to Figure 3.

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<sup>12</sup> Prof. Primas was originally trained as a chemical laboratory technician, and functioned as such before establishing himself as a leading experimental and theoretical chemist. (Atmanspacher 1999)

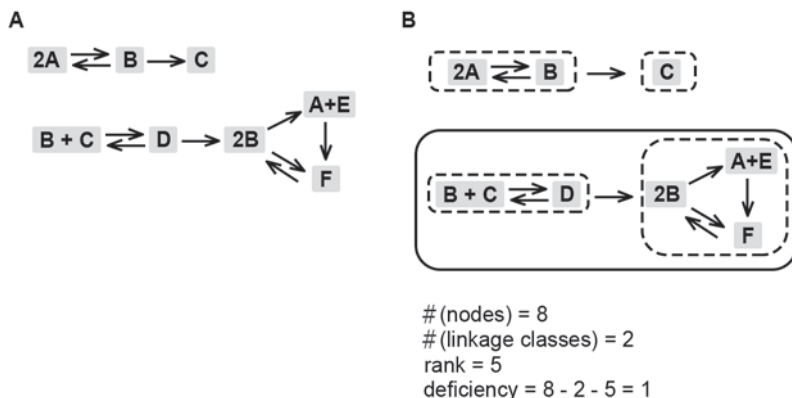


Figure 3. A reaction network that exhibits absolute concentration robustness. Taken, with permission, from Shinar 2010.

- *Nodes* are distinct combinations of chemical species that stand at heads and tails of reaction arrows. (Each node appears only once in a standard network diagram.) In the figure there are eight nodes: 2A, B, C, B+C, D, 2B, A+E, and F.
- Sets of mutually-linked nodes are known as *linkage classes*. There are *two* linkage-classes in the network shown, as indicated by the solid lines on the right half of Figure 3.
- A group of nodes constitute a *strong linkage class* if there is a path of directed arrows from one node to each of the others and also from each of the others to that one (dashed lines in the figure).
- A strong linkage class is *terminal* if none of its nodes involve an arrow leading to another linkage class. In the figure, both C and the class [2B, A+E, F] are terminal classes. There are two non-terminal classes, each of which has two nodes.
- The *rank* of a network is the maximum number of *independent* reactions the network contains. Only *five* of the ten reactions shown in Figure 3 qualify as being independent.
- The *deficiency* of a network is an integer index obtained by subtracting both the number of linkage classes and the rank from the number of nodes. For the network of Figure 3 the deficiency is one, because there are eight nodes, two linkage classes, and the network has a rank of five.
- A system is said to have “absolute concentration robustness in species S” if the system admits a positive steady state and if the concentration of S is the same in all positive steady states.

The theorem Shinar and Feinberg established by *a priori* reasoning is:

Consider a mass-action system that admits a positive steady state and suppose that the deficiency of the underlying reaction network is one. If, in the network, there are two non-terminal nodes that differ only in species  $S$ , then the system has absolute concentration-robustness in  $S$ .

In the network shown in Figure 3 there are two non-terminal nodes ( $B+C$  and  $B$ ) that differ only in species  $C$ . The theorem therefore requires that the network shown exhibits robustness in the concentration of species  $C$ . That is, over a wide range of the other concentrations involved, the concentration of  $C$  will have the same value. This theorem correctly rationalizes approximate concentration robustness that has been experimentally observed in several biochemical networks. Presence of concentration robustness in a network favors incorporation of that network as a reliable component part of larger dynamic systems.

In some biochemical systems where the concentration-robustness theorem applies, the key species is a single bifunctional enzyme that acts as a catalyst for two quite-different reactions. Presence of such a bifunctional catalyst in a reaction network is a good indication that the network may display concentration robustness. Remarkably, a naturally-occurring example of such a bifunctional catalytic species has recently been found in ancient organisms. Say and Fuchs (2010) report discovery of a bifunctional glycogenic enzyme, “fructose 1,6-bisphosphate aldolase/phosphatase.” This substance catalyzes the combination of two small molecules to produce the six-carbon sugar fructose 1,6-bisphosphate. Simultaneously the same molecule also catalyzes removal of one phosphate group from that rather unstable initial product to yield a much more stable fructose monophosphate. (Please see Figure 4 below) This new type of enzyme has been found to be contained in “virtually all archaeal groups”—including many ancient biological species that have high-temperature “chemoautolithotrophic” metabolism. These are critters of exceedingly ancient lineage that live at temperatures close to or above the boiling point of water and fulfill their food requirements by chemically degrading rocks.

Current theories of the origin of life at sites of undersea volcanic activity (e.g., Smith and Morowitz 2005, Earley 1998a) postulate that, at or just prior to the origin of life, previously-existing endothermic reaction-networks that produce six-carbon sugars from three-carbon precursors (using geologic energy for glycogenesis) *reversed their direction of operation* to yield exothermic reaction-networks that use six-carbon sugars to produce three-carbon products (in energy-releasing glycolysis) and thereby made biological activity possible. This quite novel bifunctional catalyst was discovered in the most ancient currently existing organisms,

has characteristics conducive to concentration robustness, and brings about an essential step in the postulated glycogenetic mechanism. Taken together these facts have been interpreted to suggest that this enzyme may be a “dynamic fossil” that preserves information relevant to the dawn of proto-biology. (Gunawardena 2010) This specific suggestion is speculation. What is not speculation is that *closure* of dynamic networks of chemical processes, what we here call *Closure Jacques Cauvin*, did play a central role in the origin of life, and also in the beginnings of each of the myriad more-complex dynamic coherences that now characterize our world.

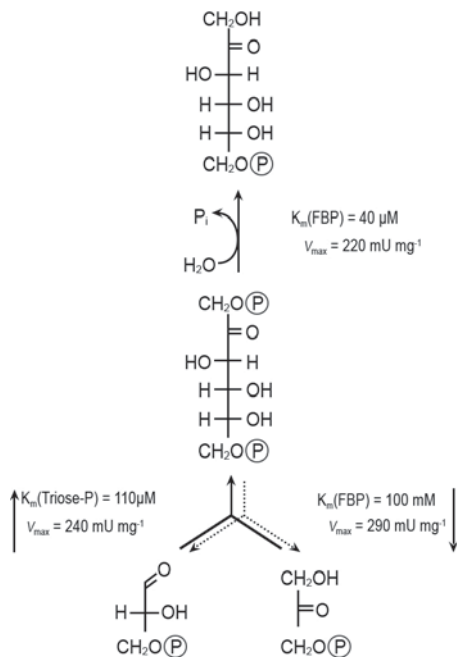


Figure 4. Action of bifunctional fructose 1,6-bisphosphate aldolase/phosphatase. Taken, with permission, from Say 2010.

Each coherent structure of processes necessarily exchanges materials and energy with the rest of the world, and also must increase the global *rate of entropy production*. These characteristic interactions of such open-system “*dissipative structures*” have important causal consequences (Earley 2006).

In *The Birth of the Gods and the Origins of Agriculture* (1994, 2000) anthropologist Jacques Cauvin explored how prior changes in concepts



and social practices *made possible* initial development of agriculture, and thereby grounded the flourishing of subsequent human cultures. On this basis, we designate any mode of *closure of networks of processes* that makes further network-formation possible as “*Closure Jacques Cauvin*.” Systems that show concentration-robustness (including those involving the ancient bifunctional enzyme) are examples of this type of closure. Elsewhere, I consider such systems in terms of “Process Structural Realism” (Please see my article “An Invitation to Process Philosophy,” in this volume, and Earley: forthcoming, 2008a, 2008b, 2006, 2003b, 2003d).

Cauvin’s insight has been developed by recent studies based on evolutionary network theory (Atran 2010). These have clarified how human agents have themselves been shaped by relational networks—at the same time that each of those networks has been created by the choices of those same agents (and of others like them). Marjorie Grene (1978) observed:

We do not just have rationality or language or symbol systems as our portable property. We come to ourselves within symbol systems. They have us as much as we have them.

One finding of Atran’s recent (2010) research that may be surprising is the conclusion that transmission of a conceptual system is greatly *enhanced rather than impeded* if that scheme of thought involves some “counterintuitive” (i.e., incredible) concepts. Such propositions have surely played essential roles in major advances in human evolution. [Perhaps the widespread acceptance of the counterintuitive doctrine that objects are merely “bundles of properties” can be understood on this basis.] Human individuals do develop their identities *within* social and technological network-structures—but the actions of those persons (along with other factors) *constitute* those same networks (e.g., Harré 1999).

## Closure and Epistemology

Much current philosophy of science seems to be subject Putnam’s (2004, p.84-85) objection:

Once we assume that there is, somehow fixed in advance, a single ‘real’ a single “literal” sense of “exist”—and, by the way, a single ‘literal’ sense of identity—one which is cast in marble and cannot be either contracted or expanded without defiling the statue of the god, we are already wandering in Cloud-Cuckoo Land.

Taking such attacks seriously supports the conclusion of Atmanspacher & Primas (2005):

... States and properties of a system which belong to an epistemic description in a particular domain can be considered as belonging to an ontologic description from the perspective of another domain.

This move would be quite consistent with Michel Bitbol's (1998) transcendental epistemology<sup>13</sup>:

objects are no longer regarded as constituents of our experience but rather as (i) potential aims for our research and resolution and (ii) elements in our strategy for anticipating the outcomes of our activities.

The characteristics of the objects that philosophers usually discuss (such as roses, statues, tennis balls) depend on the chemical closures that involve the components of those entities, and also on closures (e.g. decisions) of other sorts (involving plant breeders and gardeners, sculptors and their patrons, and committees of the US Lawn Tennis Association).

Each of the three types of closure described in this chapter corresponds to a transition in *topology of description*. Louis de Broglie clarified (for his time) how coherence of electrons and nuclei *constitute* atoms—basic units of “an ontology.” Henri Poincaré demonstrated how new topologies (ontologies) result from cooperative action of molecules. Jacques Cauvin showed how the invention (or discovery) of human conceptual systems *enabled* (“afforded”<sup>14</sup>) yet further evolutionary advance. Each of these three sorts of closure *makes additional kinds of human understanding possible*—therefore each of them corresponds to a major transition in *epistemological* possibility.

As *Closure de Broglie* provides the basis for intra-molecular processes and super-molecular coherences, and *Closure Poincare* grounds the ontological change brought about by highly cooperative inter-molecular interactions, so *Closure Cauvin* make possible evolution of still more-complex dynamic coherences of *processes*—including ourselves and our cultures. Undoubtedly other modes of closure exit. The important point is that causal functions (“properties”) of items depend, in every case, on underlying *closure of relationships*.

Chemistry—“The Central Science”—can provide students and other young people excellent opportunities for technological participation in the

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<sup>13</sup> This approach is closely related to Rom Harré's physical-science-related “policy realism.”

<sup>14</sup> Please see Rom Harré's paper in this volume.

development of future societies. In addition, Philosophy of Chemistry can significantly increase properly philosophic understanding, thereby contributing to humanizing the ongoing evolution of dynamic structures—not only those of a technological sort but also high-level conceptual systems, and the large-scale social arrangements they eventually generate.

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# AN INVITATION TO CHEMICAL PROCESS PHILOSOPHY

JOSEPH E. EARLEY, SR.

## 1. A Cordial Invitation

“Process philosophy” has resources that would be useful in philosophy of chemistry. This approach would particularly appropriate for dealing with questions involving time-dependent self-organization in far-from-equilibrium open systems. (Such spontaneous generation of coherent dynamic structure is of central importance in many fields including chemical engineering, systems biology, and economics.)

Not long ago a single rather coherent and widely shared point of view dominated discussions of philosophy of science. Many scientists and philosophers believed that natural processes would soon be well understood in terms of few types of microscopic “elementary” particles—and, correspondingly, that a mainly-analytic style of philosophy would ultimately resolve all (or most) important questions. However, recent developments—both in philosophy and in science—have called main features of that former near-consensus into question. Now, several philosophical traditions contribute to treatments of the mutual influences of science and philosophy. “Process Philosophy”—a science-related philosophical approach largely based on contributions of Alfred North Whitehead (1867-1947)—was widely discussed in the mid-twentieth century, and deeply influenced such scientists as C. H. Waddington (1905-1975)—the founder of “systems biology.” The process-philosophy point of view has not been prominent in recent philosophy of science but it has resources to address some main current problems. Please consider this chapter as an invitation to consider looking into this approach for dealing with contemporary questions in the philosophy of chemistry.



## 2. The Philosophy of Organism

Whitehead began his academic career as a member of the mathematics faculty of Cambridge University. With his former student Bertrand Russell, he wrote *Principia Mathematica* (1910-1913)—to set out a *strictly logical* basis for mathematics. Apostolos Doxiadis (2009) shows (effectively using a graphic-novel format) how that book inspired much of the fundamental intellectual progress that was made in the early twentieth century—even though it fell well short of achieving its original goal. From 1910 to 1925, Whitehead taught mathematics and physics (and provided highly significant academic leadership) in London, first at University College and then at Imperial College. During this period he published important work on philosophy of science and also on education. He then accepted an invitation to join the philosophy faculty of Harvard University—from which he retired in 1937.

While in Massachusetts, Whitehead developed a complex and wide-ranging philosophic outlook that he named “the philosophy of organism.” Ideas characteristic of his first years at Harvard were set out in several books including *Science* and the *Modern World* ([1926] 1967—hereafter, SMW), subsequently developed into a complex formal system in *Process and Reality* ([1929] 1978—hereafter, PR), and later applied and further refined in less-technical works such as *Adventures of Ideas* ([1933], 1967—hereafter, AI). In the preface to his major work (PR xii), Whitehead states: “I am ... greatly indebted to Bergson, William James, and John Dewey. One of my preoccupations has been to rescue their type of thought from the charge of anti-intellectualism, which rightly or wrongly has been associated with it.”

Many philosophers have published introductions to Whitehead’s thought: *Thinking with Whitehead* (2011) (by Belgian chemist and philosopher Isabelle Stengers) will be of particular interest to chemists and philosophers of chemistry. That work is also available in the original French as *Penser Avec Whitehead*, 2002, as is a related later work (Debaise 2006), and a multi-author collection (Stengers 1994). With regard to reading Whitehead’s original work, it would be prudent to start with the less-formal works (AI or SMW) and only later to turn to the more-technical exposition in PR.

### 3. An Introductory Sample

Many of the main themes of Whitehead's thought that seem especially pertinent to chemistry can be recognized in a single passage (SMW, pp. 93-94) that is quoted (in italics) below. [My comments are inserted in brackets.]

*One all-pervasive fact, inherent in the very character of what is real, is the transition of things, the passage one to another.*

[For Whitehead, what is fundamentally important is process, change, evolution—but all change derives from the origination of coherence. “Becoming” is more basic than is “being.” (Earley 2008c)]

*This passage is not a mere linear procession of discrete entities. However we fix a determinate entity, there is always a narrower determination of something which is presupposed in our first choice. Also there is always a wider determination into which our first choice fades by transition beyond itself.*

[Any and every item that can be identified (by humans or otherwise) is made up of less-inclusive components. Also, each and every item is itself a component of one or more more-inclusive items. This is an approach to the theory of parts and wholes (“mereology”) that is quite different from the Standard Extensional Mereology (SEM) which is generally accepted by current philosophers (Simons 1987)—but Whitehead's insight is more consistent with contemporary chemical understanding than is SEM (Harré 2011).]

*The general aspect of nature is that of evolutionary expansiveness. These unities, which I call events, are the emergence into actuality of something. How are we to characterize the something which thus emerges? The name 'event' given to such a unity, draws attention to the inherent transitoriness, combined with the actual unity.*

[Items are “events” rather than “substances”—they all and always come to be and promptly perish—while they all participate in continual evolutionary development which is a main characteristic of the world.]

*But this abstract word cannot be sufficient to characterize what the fact of the reality of an event is in itself. A moment's thought shows us that no one idea can in itself be sufficient. For every idea which finds its significance in each event must represent something which contributes to what*

*realization is in itself. Thus no one word can be adequate. But conversely, nothing must be left out.*

[Every aspect of items or events that we can identify provides us with basic insights of wide (even general) applicability—but our best understanding is always partial and incomplete.]

*Remembering the poetic rendering of our concrete experience, we see at once that the element of value, of being valuable, of having value, of being an end in itself, of being something which is for its own sake, must not be omitted in any account of an event as the most concrete actual something. "Value" is the word I use for the intrinsic reality of an event. Value is an element which permeates through and through the poetic view of nature. We have only to transfer to the very texture of realization in itself that value which we recognize so readily in terms of human life. This is the secret of Wordsworth's worship of nature. Realization therefore is in itself the attainment of value.*

[This selection occurs near the end of a chapter of SMW that deals with "The Romantic Reaction" against Newtonian science. Poetry generally concerns specific situations in which a poet discerns some worth, significance, or interest. Whitehead designates as "value" whatever accounts for the coherence of any item or event, in so far as it is, in fact, one item or event: he assigns a new (and quite technical) meaning to the common English word "value." In his view, every item or event whatsoever has intrinsic value—thus he avoids difficulties associated with the usually-presumed fact/value opposition.]

*But there is no such thing as mere value. Value is the outcome of limitation. The definite finite entity is the selected mode which is the shaping of attainment; apart from such shaping into individual matter of fact there is no attainment. The mere fusion of all that there is would be the nonentity of indefiniteness.*

[Whitehead endorses the ancient doctrine that there is nothing that exists "in general"—each real item must be a specific something.]

*The salvation of reality is its obstinate, irreducible, matter-of-fact entities, which are limited to be no other than themselves. Neither science, nor art, nor creative action can tear itself away from obstinate, irreducible, limited facts. The endurance of things has its significance in the self-retention of that which imposes itself as a definite attainment for its own sake. That which endures is limited, obstructive, intolerant, infecting its environment with its own aspects.*

[All action, human or other, must take account of the fact that specific enduring items continually reassert their defining characteristics, and thereby each and all of them influence future items and events.]

*But it is not self-sufficient. The aspects of all things enter into its very nature. It is only itself as drawing together into its own limitation the larger whole in which it finds itself. Conversely it is only itself by lending its aspects to this same environment in which it finds itself.*

[It is never possible to isolate a specific item or event: things are all interconnected in many ways both simple and complex. The reality and identity of any event or item depends both on its components and their inter-relations and also on whatever it may comprise. Late-twentieth-century authors emphasized the dependence of composites on their components but neglected the importance, for the components, of the composites which they comprise.]

*The problem of evolution is the development of enduring harmonies of enduring shapes of value, which merge into higher attainments of things beyond themselves. Aesthetic attainment is interwoven in the texture of realization.*

[Evolution—broadly understood—continually leads to “concrecence” of ever-new modes of coherence, each of which involves the achievement and also the “enjoyment” of value: and each is an accomplishment that is “felt by” (influences) subsequent coherences. Many such “levels of reality” mutually influence each other—interference among values pertaining to diverse levels may lead to disruption, and thus to loss of coherence.]

*The endurance of an entity represents the attainment of a limited aesthetic success, though if we look beyond it to its external effects, it may represent an aesthetic failure. Even within itself, it may represent the conflict between a lower success and a higher failure. The conflict is the presage of disruption.*

[Decay (or over-development) of a component may interfere with or destroy an upper-level coherence. Conversely, failure (or excessive success) of a higher level may threaten continued existence of some components. But, as the first sentence of this selection points out, change is a main and ubiquitous feature of the world.]

#### 4. Whitehead's Philosophical Heresy

Natural human languages function as if all items fall into one or the other of two great classes—often designated as “substances” and “attributes”—or, alternatively, as “particulars” (individuals) and “universals” (properties and relations). Historically, most philosophers have adapted their conceptual systems to this linguistic usage, and most do so now. In contrast, Whitehead maintained (PR 18) that “Actual entities—also termed actual occasions—are the final real things of which the world is made up. There is no going behind actual entities to find anything more real. ...The final facts are, all alike, actual entities; and these actual entities are drops of experience, complex and interdependent.” Each actual occasion emerges from “prehensions” (“feelings”) of antecedent actualities which feelings are progressively unified (this is technically called “concrescence”) with reference to a “subjective aim”—a “form of definiteness” (an “eternal object”). The “final real things” all perish as they come to be—they are definitely not “substances” with “properties.”

Although actual occasions do not persist, when several successive actual occasions share the same defining subjective aim they constitute a “society” with “personal order”: such coherences may endure for long periods—although none of the actual occasions that comprise them continues. Whitehead remarked (AI 206): “The Universe achieves its values by reason of its coordination into societies of societies, and in societies of societies of societies.” Societies, however complex and important they may be, are nothing apart from the actual entities that comprise them. Whitehead's system differs from other current philosophical approaches in truly fundamental ways. Whitehead challenged basic and widely shared assumptions, by taking time fully seriously (as Prigogine later recommended). One reason that Whitehead is not widely quoted in philosophy of science is that his view of time confuses and/or repels a number of philosophers. However, rejection of the substance-attribute approach opens up new opportunities for dealing with philosophical problems that are important for contemporary culture. Although Whitehead takes great care not to provide examples of specific actual entities, he does apply his conceptual scheme to important philosophical problems (particularly in AI).

## 5. Process Structural Realism

The fundamental outlook (“idea of nature,” “worldview,” “*weltanschauung*”) that emerges from (and is required by) the most active areas of current science is intrinsically temporal—processes are of central importance. Classical thermodynamics largely concentrates on systems that are at, or very near to, equilibrium: thereby it avoids complications that arise when time-dependent processes are considered. But most systems of interest to practicing chemists and chemical engineers are kinetically determined, rather than thermodynamically determined—and often remain far from equilibrium. It is essential for chemists and chemical engineers to deal with rate-processes. A related situation obtains in philosophy, but is often not recognized. Philosophers usually discuss questions on a synchronic (instantaneous) rather than a diachronic (recognizing temporal aspects) basis—even though they rarely make that choice explicit. (Remarkably, systems of temporal logic, involving such concepts as “until,” were not developed until the 1950s.) Unfortunately, it turns out that conclusions reached on a synchronic basis often are quite wrong.

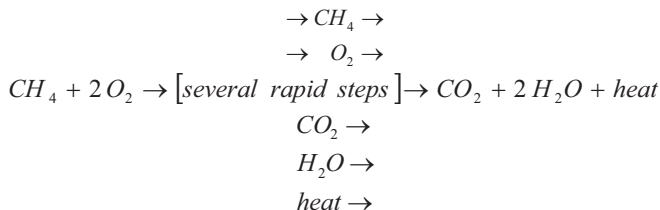
The composition and structure of chemical samples do not depend solely (and usually not even mainly) on the energetics of the instantaneous interactions between their components—as philosophers often routinely assume. The determining importance of rate processes and other contingent historical events for chemistry must be taken into account. Whether a particular sample that analyzes as  $C_3H_4$  is actually allene, cyclopropene, or methylacetylene is determined by the processes that were involved in the generation of that sample—and cannot be calculated by any method that ignores that history (Earley 2012).

Internal balance characterizes everything that endures. Ordinary material objects involve equilibration of attractions between and among components (which tend to compact each entity) and mutual repulsions (which keep parts separate). At all temperatures, every part is in motion. Maintaining the attraction-repulsion balance requires that all such motions be oscillatory—that is, a closed set of states of the composite must repeatedly occur. Coherences often interact with others—and frequently bring about rearrangements of components and thereby produce new types of order. Each such creative process involves both the coming-to-be of new coherences and the dissolution of old ones. Chemical reactions are especially well-understood examples of this type of change—but analogous interactions are ubiquitous (e.g., in biology, psychology, and economics).

Usually, processes use up their starting materials and gradually slow down. However, some processes continually get faster—because, for instance, they produce greater quantities of their reactants than they destroy. Such “autocatalysis” often leads to explosion: however, in open systems, autocatalytic processes may combine with interactions that reduce the effectiveness of autocatalysis so as to achieve a balance—and oscillations in the amounts of reactants and products then may persist over long times. Every “organism” (biological or other) involves many such open-system “homeostatic” arrangements. Many chemically important entities are self-organizing open-system coherences that are made up of processes (Earley 2006). This type of generation of long-lived dynamic coherence is an example of the genesis of what Whitehead (PR 203-207) called “social order.”

A steady flame is not a collection of things—it is a persistent coherence of chemical reactions and physical processes (e.g., Scheme 1)—what Ilya Prigogine called a “dissipative structure” (Kondepudi 2008). The combustion reaction operates faster at higher temperatures. Since that reaction produces heat that increases the temperature of the reaction mixture, combustion is autocatalytic (goes faster as it proceeds). As temperature rises, diffusion of heat out of the system increases and moderates the autocatalysis. In favorable cases, input of reactants and exit of heat and product molecules may reach a balance, to yield a steady flame. So long as fuel and oxidizer enter and combustion products escape, the flame may persist in (more or less) the same temperature and shape. Such a steady flame might function (as signal or source of heat) in yet other coherences. Steady flames demonstrate an important type of “societal” order: we consider a stable flame as a Whiteheadian “society.”

*Scheme 1.* A minimum set of constituent processes for a steady flame. The first two lines describe entry (and exit) of fuel and oxidizer into (and from) a reaction zone. The last three lines describe the exit of products from that region.



A steady flame is a complex unit in which diverse processes (including chemical reactions and fluxes of heat and molecules from and to the surroundings) combine to yield a set of relationships that is characteristic of that enduring coherence. The balance achieved by the processes provides the “form of definiteness” of a unified agent. A specific closure of relationships (a dynamic structure) thereby individuates that coherence as what it is and also (concurrently) grounds the relations of the coherence with the external world. Successor members of that society would inherit the same (or very nearly the same) non-mysterious structure from predecessors. That is to say, **when a group of processes achieves such closure that a set of states of affairs recurs continually, the effect of that coherence on the world differs from what would be the case in the absence of that closure.** Such altered effectiveness is an attribute of the system as a whole, and would have consequences. Whenever a network of processes generates continual return to a limited set of states of affairs, the system may function as a “whole”—with respect to appropriate interaction partners. [For further development of related ideas please consult my other paper in this volume: “Three Concepts of Chemical Closure and Their Epistemological Significance.”]

The causal powers of such coherent aggregates are indeed just the powers of the constituents “acting in concert.” However, the components act in concert in the specific way they do only because of their inclusion in the closed set of interactions that defines the coherence. The causal powers of the coherence defined by that closure are not redundant. Combinations of processes produce effects that are not simply attributable to the constituent processes. Whenever such efficacy is important in some discourse, non-redundant structural causality warrants recognition of those coherences as ontologically significant for that discourse. (There is no “God’s-eye view” that is not limited in this way.) This approach is a variety of “structural realism” (Bokulich 2011) and also a kind of process philosophy. The designation “Process Structural Realism” (PSR) seems appropriate (Earley 2008a,b).

Process philosophy deals with questions (especially concerning the temporal origin and effects of dynamic non-equilibrium coherences) that mainstream philosophy has systematically ignored for several centuries. Such formerly invisible issues are now showing up in many areas of contemporary thought (e.g., Bowles, 2011). Application and further development of process-philosophy approaches could contribute to significant (and perhaps widely important) progress for philosophy of chemistry.



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# ABOUT THE CHEMICAL EXPERIMENT\*

JOSÉ A. CHAMIZO

## 1. About Chemistry Laboratories

In laboratories, spaces dedicated to practical work, rather than theoretical research the activities conducted there for thousands of years have been considered of less intellectual value. The Latin word *aborare* remind us of manual labour conducted by slaves in both the Roman Empire and the Greek cities. The 17<sup>th</sup> Century English philosopher T. Hobbes indicated the low status of those engaged in practical work: grocers, gardeners, blacksmiths or mechanics. Those who assumed that money (in order to buy better materials and / or equipment) could give them knowledge were wrong. Since the earliest times in History and especially from the Middle Ages on, the preparation of medicines, the manufacturing of soaps, pigments, glass, ceramics, explosives and metal mining were practical activities far from the philosophical thinking and developed around markets and public places. These activities were carried on by skilled craftsmen who learnt their trade by apprenticeship imbued with a certain amount of religious ideas. However, even since that time was recognized the most important feature of a laboratory: its isolation from everyday life. Chemical laboratories that predated physics' labs for almost two centuries first accomplished this. As indicated by Crosland (2005, p. 238-9):

To be dignified by the title 'laboratory', a dedicated space, whether a room, cellar, or whole building, has to be fitted up especially for the purposes of practical science ... Given this more rigorous definition of a laboratory, the first laboratories were the laboratories of the alchemists ... The basic facility required for practical chemistry was a source of heat. In alchemical laboratories, there would be one or more furnaces, ideally together with a fuel store, a water supply, preferably complemented by a sink, flasks, retorts, and other apparatus, and a variety of labelled chemicals

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\* A preliminary version was presented in the 2010 *Summer Symposium of the International Society for the Philosophy of Chemistry*, Oxford.

reagents. As we have previously indicated, it was usual for alchemical laboratories to have a number of different types of furnace, providing ascending degrees of heat, ranging perhaps from a gentle fire with a water bath to a reverberatory furnace. Distillation would usually be carried out at an intermediate temperature, although, of course, the concept of temperature really had to wait until the eighteen century.

Thus since the 17<sup>th</sup> Century access to a permanent heat source and tap water existed for the space that today is recognized anywhere in the world as a laboratory. By early 19<sup>th</sup> Century chemical laboratories had integrated the newfound electricity that H. Davy so effectively used in England to isolate many of the alkali and alkaline earth elements.

The equipment and reagents in chemical laboratories were crafted products, manufactured and prepared locally. They were expensive according to the letters that Cannizzaro wrote in the 19<sup>th</sup> Century to his colleagues in different parts of Italy, so that they could exchange items among themselves (Cerruti, 1998). The double trade of chemicals and equipment through the 18<sup>th</sup> and 19<sup>th</sup> Centuries in many European countries is well documented (Brock, 1992) and in a one-way direction with the American colonies. Spreading of equipment and reagents also meant the spreading of practices and ideas. It is worth stressing that the 17<sup>th</sup> Century laboratories built their equipment with two main objectives: first, for chemistry research itself; and then, to teach (Brenni, 2010). Some of the equipment used by A. Lavoisier had this latter purpose (Russell, 1985). For example the mass production of balances began in London only until mid-19<sup>th</sup> Century, not long before Bunsen, in Germany, invented his famous burner-lighter.

The laboratory of Justus von Liebig, who invented the bulb apparatus to measure the carbon content in a sample -a device that helped to transform organic analysis and grounded the systematic study of fertilizers in Giessen- was perhaps the first space designed specifically for the experimental teaching of chemistry. Until mid-1830, this was a marginal science at German universities. Its importance there started to grow as did the demand for scientists in this area of knowledge by the burgeoning pharmaceutical industry that was in urgent need of them. Liebig was a precursor in this regard as the first designer of pedagogy focused on chemistry, requesting financial support from the German government to implement it. Following his idea: “the job of the scientist was to ask questions which could be answered, and this meant doing definite experiments rather than wasting capital and power in vague trials”. In his lab, youngsters were trained on the basis of experimental methods for chemical research, analysis and synthesis. The teacher posed a problem

and several students investigated, according to their prior knowledge and criteria, different ways to solve it. The advanced students helped the beginners, so their number could be -as indeed was- much greater than elsewhere. That's how Liebig's disciples got most of the job vacancies at the universities in Germany and abroad.

In brief, laboratories for the research or teaching of chemistry took form long before those from other sciences as did the equipment and reagents used to work. Yet historians have paid little attention to this matter. Holmes (2000, viii) suggested that:

One reason for the historical neglect of chemical apparatus has been the dearth of material evidence. Chemical apparatus, for the most part, has been made of glass, earthenware, and stoneware. It is seldom signed and seldom is especially beautiful; therefore, it is of much less appeal to collectors than the astrolabes or microscopes. More than most laboratory equipment, chemical apparatus is disposable. Platinum crucibles are melt down, to be turned into a new instruments or components. Glass breaks and, after it has been used several times in stressful conditions, it becomes even more fragile and then can't survive long.

In the activities that have become what we know now as chemistry it is possible to trace its humble origins. Manual work originally performed by slaves and craftsmen, isolated from the deep meditations would summon philosophers, made of fragile materials that withstood the ravages of time and in secluded areas of the multitudes. All those activities have experimentation in common.

## **2. About Experiments and Apparatus**

It is a common idea, to think science is experimental. However this is only accurate when it comes to chemistry. The first voluntary interventions that humans did on their surrounding world involved fire thereby transforming it... and so has been the case until today. On the other hand, astronomy and biology have developed from observations, modelling and reasoning, while in physics the so-called "thought experiments" (more than experiments, imaginary or mental exercises that therefore do not appeal to an intervention in the world or hence to a laboratory) have been important (Snookes, 2006).

There are many definitions of what an experiment is, but out of all them I will appeal to two relatively recent where the concept ceases to be subsumed passively in the realm of theory and thought:

To experiment is to create, produce, refine and stabilize phenomena (Hacking 1983, p. 230).

An experiment is the manipulation of apparatus that is an arrangement of material stuff integrated into the material world in a number of different ways (Harré, 2004, p. 175).

It can be understood from these quotations that experimental work not only prepares the experiment, design and construct devices (there is an important tradition within chemistry in this sense, Knight, 1995); it creates the phenomena as well. Here is important to note that there has been a customary way of conceiving scientific activity and understanding the phenomena found in nature. This has led to a delicate characterization of what is a discovery which, according to Achinstein (2001), is reduced to three factors: ontological (the thing discovered must exist); epistemic (the discoverer must be in certain knowledge-state towards the discovery); and priority (this state must be a first). However, new positions taken up by technoscience (Pickestone, 2000, Echeverria, 2003) suggest that scientists create phenomenon that later become centrepiece's of their theories. Here is relevant to recall the concept of affordance, introduced by Gibson (1979) to distinguish a certain class of dispositions. They are conditional (Harré 2004, p. 188): 'If certain conditions obtain then a certain phenomenon will (probably) occur'. These conditions can be intentionally designed into the phenomenon. In the same vein Harré reminds us that Bohr already indicated that the apparatus (Harré, 2004 p.180):

... does not model the production of naturally occurring phenomena as a discharge tube might. It creates phenomena that do not occur in nature in the absence of the apparatus.

Analysis was, for Lavoisier, the operation that defined chemistry. But according to a "distinguished fellow countryman, almost half a century later, he was wrong". Berthelot's famous phrase, "Chemistry creates its own object", marks a new path in chemical practice. This was a specific desecration; the vast majority of chemists' knowledge is a creation, not a discovery, as they thought the alchemists. If analysis considers the separation and identification of the nature of the material components in substances, the synthesis is about how to put them together creating new substances. The current chemical synthesis, rather than anything else, is based on the systematic production of novelty and this is done through chemical experiment. As indicated by Schummer (2004, p. 399):

... however, the great majority of chemists actually produce new substances. That is by far the largest scientific enterprise—roughly estimated,

a third of all scientists worldwide are involved in this project. Surprisingly, no philosopher of science seems to have ever been aware of it.

### 3. About Models

Model is polysemous word; it has been used and is still used with different meanings. In this paper we continue our investigation (Chamizo, 2010, 2011) and characterize models as follows: *Models (m) are representations, usually based on analogies, which are built contextualizing a certain portion of the world (M), with a specific goal.*

In this definition all the words are important: representations are essentially ideas, but not necessarily, as they can also be material objects. Representations have no meaning by themselves. Representations are done from someone (either an individual or a group, usually the latter) that identifies them as such. An analogy is made up of those features or properties that we know similar in (m) and (M). That is built into context, referenced to a historically defined time and place that also frames the representation. Some portion of the world indicates its limited nature; models (m) are, for the world (M), partial. A specific goal establishes its own purpose, usually but not necessarily explained, and also predicted. Explanation is one of the most significant features of science (Bailar-Jones, 2002), but in some cases even though completely unable to explain, much of its prestige lies in predicting.

Models (m) are representations, usually based on analogies (Achinstein, 1987; Clement, 2008). They can be similar to that portion of the world they represent, usually simple, but not entirely, so that hypothesis can be derived (and / or predictions) and testing them. The test results provide new information on the model. There are two types of models: mental and material.

Mental models (Clement and Rea-Ramirez, 2008) are reflected representations built by us to account (explain, predict) a situation. They are the forerunners of the famous "misconceptions" (Kind, 2005) and can sometimes be equivalent.

Material models (which may be identified as prototypes) are the ones that we have empirical access to and have been built to communicate with other individuals. Material models are expressed mental models (Gilbert, Boulter and Elmer, 2000) through a specific language, such as mathematics or chemistry. When the language is expressed in symbols, we speak of symbolic material models. So those constructed mathematical equations to describe precisely the portion of the world being modelled (Mehrtens, 2004) are symbolic material models. These represent the regularities that

different scientific communities at various times in history have identified in some portion of the world (**M**). These models, known as laws, are the most common, though not the only ones, to explain in scientific tradition (Suppe, 1989). Another example of symbolic material model is the one used by chemists to represent elements, compounds and reactions (Hoffmann and Lazlo, 1991).

In addition to symbolic material models are experimental material models and iconic material models. Examples of experimental material models (Pérez-Tamayo, 2005; Harré, 2009) are male Sprague-Dawley rats used in a standardized way in biomedical research or disease, modelling action of possible remedies for them. Experimental material models are also devices or apparatus (Harré, 2004), such as the famous Urey-Miller (that allowed the generation of amino acids on the original conditions of the atmosphere) or tokomac (in which we study the fission reactions that occur in stars) with experiments carried out to simulate a particular aspect of the world (**M**). Iconic material models correspond to images, diagrams or scale-models, like a map (Tversky, 2005) or so-called 'molecular models' (Francoeur, 2001). The most famous example is the representation of the DNA molecule by Watson and Crick.

As Justi and Gilbert have shown (2002), learning to do science means that students are able to create, express and test their own models, it means modelling. Briefly, as can be seen in Figure 1, from questions about the real world, comes the construction of a first model: a mental model. This activity represents private modelling with an arrow linking the two squares and has two points because it assumes that the questions depend on the performance of the individual's mental structure, and the other defends the position following the empiricist representation which depends entirely on data obtained from the perception or consensus about the world. The second step in modelling is to express the mental model, building a material model (symbolic, iconic or experimental). Finally, the material model should be subjected to the most important test, contrast between the material model and the real world according to specific conventions in each case (for example some of the experimental material models can change the real world). It is a public observation also indicated by a bidirectional arrow because as a result of the very same observation adjustments can be made to the material model so that it fits right with the real world. The assemblage prioritizes quality of explanation and predictions made by the model. Figure 1 resumes all this to glimpse a definition of chemical experiments particularly useful for educational purposes.



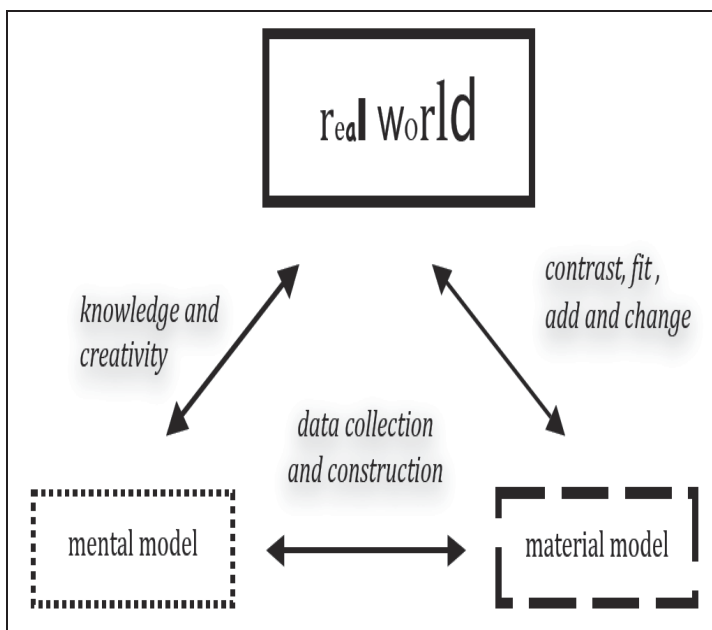


Figure 1. Relation between models and real world (in squares) with *modeling* (lines)

#### 4. About the Chemical Experiment

As indicated above, one of the three types of material models is the experimental material model. Related to this Harré has said (2004, p. 180):

The apparatus is a material model of the naturally occurring material set-up.

However, not all apparatus or experimental material models have an analogous relationship with a certain portion of the world. For example one of the most interesting moments in the history of experimental chemistry was developed in the second half of the seventeenth Century within the so-called pneumatic chemistry (Shapin & Schaffer, 1985). At the time, apparatus, experimental material models, allowed the isolation of "new" constituents of air. Hence and to be more specific, it is possible to recognize that some apparatus: i) are 'material' models; ii) create

phenomena and iii) are instruments (physically able to isolate the properties of the entities that want to use and / or to know).

If an instrument isolates the properties of the entity being studied, solvents and indicators are instruments. Cerruti (1998) recognized this and suggested a parallel between acid-base indicators and thermometers. So it is also possible to recognize that the electrochemical synthesis of sodium made by Davy in 1807 was successful because it was conducted in the absence of water. A piece of sodium behaves in a certain way with water, in another with mineral oil and in a well known different way with other substances, like liquid ammonia. Nowadays we are carrying out many chemical reactions in absence of water or gases such as oxygen, which substantially alters the products obtained. As Cerruti clearly stated (1998):

A fundamental use of certain solvents is to permit reactions between other substances that –under different conditions- would not be able to react, or would react in a different way. Thus, in many cases, solvents provide reaction media, tailored on chemist's synthetic needs: on a single laboratory bench, in otherwise equal vessels, different solvents furnish distinct environments in which the same substances have unlike interactions.

Experiments, according again to Hacking (1983) are “to create, produce, refine and stabilize phenomena”, indicating that the synthesis of a particular chemical, which as stated above is the most productive scientific enterprise, could be achieved with a solvent, but not with another. It follows an important characterization (Cerruti, 1998):

Phenomena are generally accepted, and philosophically discussed, as the aims and the result of experiment in physics; in general substances are the aims and the results of the most important experimental practices in chemistry.

Chemists, roughly a little over three million people around the world, make new substances. The number of substances and their commercial applications has grown dramatically over the past 200 years, from a few hundred in 1800 to over 56 million today, of which approximately 43 million are traded. The synthesis of new chemical compounds makes this the most productive science. Schummer (2006) indicates that in 2000 Chemical Abstracts, the database that provides information on most publications regarding this discipline, reported that the number of chemistry publications alone amounted for almost the same number of all the other sciences together, Figure 2.

Any person reviewing a journal of chemical research will find that the "experimental section" is very similar. It largely comprises the couple of

*synthesis* and *analysis* (Bachelard, 1976) or: performing chemical reactions in order to form new products, including their isolation and further processing, and investigating various properties of the new products. As Harré said (2004, p. 189): *what is afforded would not have existed without human action to bring it into being*. From the above it is possible to advance the following definition:

The chemical experiment creates, in an apparatus, a phenomenon (substance) using solvents as instruments (physically able to isolate the properties of the entities that want to use and / or to know).

Besides as has been considered, in reviewing the learning of chemistry in a laboratory environment (Nakhaleh, Polles and Malina, 2000, p. 85):

Research examining the concept of affordances is critical if we are to build a science of distributed intelligence and a more flexible design orientation to the practice of education.

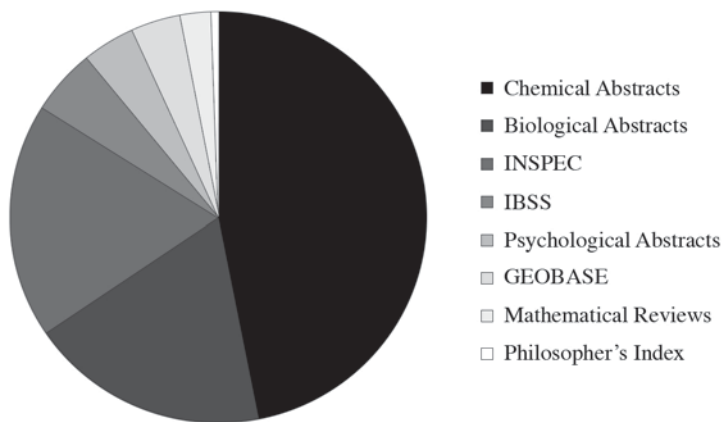


Figure 2. Number of publications (articles, books, patents, etc) indexed in major bibliographic databases in 2000. Data in thousands: CA 899, BA (biology, biochemistry, biotechnology, experimental medicine, pharmacology, agriculture, veterinary, and medicine) 360, INSPEC (physics, electric engineering, electronics, computer science, and information technology) 350, IBSS (sociology, economics, and political science) 100, GEOBASE (earth sciences) 74, MR (mathematics) 47, PI (philosophy) 10.

## Conclusion

Despite its humble origins, chemistry, using apparatus, creates a *phenomenon (substance)* and becomes the most productive science. It is possible to recognize that the word apparatus, in the context of the chemical experiment, has three different meanings: are 'material' models, create phenomena and are instruments and... *at the deeper layers of scientific work there are no transparent windows on the world, as it would be, did the apparatus not exist* (Harré, 2004, p. 189).

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# SUSTAINABLE CHEMISTRY

LAURA MAXIM AND ISABELLE RICO-LATTES

## Summary

One of the major problems in contemporary chemistry is how to integrate social and regulatory concerns about sustainable development into research and innovation practices. In order to incorporate environmental concerns, chemists adjust to new concepts and research practices, to which they assign names like “green chemistry”, “sustainable chemistry”, or “ecological chemistry”.

This chapter is written as a dialogue between Isabelle Rico-Lattes and Laura Maxim. Isabelle is a researcher in experimental chemistry; Research Director at CNRS; and Director, since its creation in 2006, of the Interdisciplinary Programme<sup>1</sup> “Chemistry for Sustainable Development”. Laura is a researcher in social sciences, who analyses patterns of research and innovation in sustainable chemistry. This dialogue focuses on interdisciplinarity, which is one of the main components of sustainable chemistry. Studies of the current methods for producing scientific knowledge in chemistry and the resulting answers to concerns related to sustainable development must address how researchers practice interdisciplinarity. Using this approach to examine the current transformations in chemistry additionally benefits from the theoretical basis that already exists in the vast literature on interdisciplinarity.

After a brief introduction to the theory of interdisciplinarity, which we will use as model for our analysis (section 1), we will address the question of the need for interdisciplinarity in sustainable chemistry (section 2). Section 3 illustrates the contribution of different disciplines to sustainable chemistry, using an empirical example - the interdisciplinary programme “Chemistry for Sustainable Development” (CPDD) led by Isabelle Rico-Lattes. The exchanges between disciplines necessary to produce

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<sup>1</sup> “Interdisciplinary programmes” are funding programmes internal to the National Center for Scientific Research (CNRS). Their purpose is to initiate small-scale interdisciplinary collaborations, with potential to grow into larger projects.

interdisciplinary work can only succeed under certain practical conditions. We will discuss how sustainable chemistry is confronted with these questions, which are related to the availability of financial and institutional support (section 4), the ability to overcome communication problems between the teams involved (section 5), and the possibilities for promoting results, both in the researchers' career and in industrial applications (section 6). We conclude in section 7 by evoking one of the main challenges for sustainable chemistry.

## 1. The Study of Interdisciplinarity: State of the Art

**LM:** I will start by briefly introducing the concept of interdisciplinarity, as it is defined in the literature. This introduction will then allow us to analyze the different components and conditions of interdisciplinarity, as practices of knowledge production<sup>2</sup>, for the particular case of research in the emerging field that is presently called “sustainable chemistry”.

It is now well known that different interdisciplinary work shares common features across both the disciplines and subjects involved in a project. The literature on interdisciplinarity has increased considerably since the 1970s. Chubin et al. (1986) found the first published work on interdisciplinary research—a 1951 paper outlining the issues encountered during a collaboration between an anthropologist and a psychiatrist. After 1969, the number of published articles about interdisciplinary works increased significantly, doubling between 1969 and 1972, increasing an additional 120% between 1973 and 1977, and another 95% between 1978 and 1982. Whereas the first research focused on educational programmes,

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<sup>2</sup> We use this term according to Vinck (2000), who defined “practices” as “effective ways of doing” (pp. 10) in research, which can be characterized in the specific case of interdisciplinary research using three elements: the epistemological framework, the devices, and the cooperation instruments. The epistemological framework refers to the conceptual basis of an interdisciplinary research project, that allows discussion of institutional stakes related to the career of the researchers involved, the scientific objectives of the collaboration, the methods to use, the research temporality of each participant, the way of formulating the research subject and the nature of the requirements, language and result formalization. The devices can concern the institutional setting of the interdisciplinary research (e.g., research group, thematic school, etc.), the ways of legitimating the scientific production (e.g., journals), and the rules of the game (e.g., concerning the industrial property, the legitimacy to talk or not in the name of a group, etc.). Finally, the instruments refer to intermediary objects that will serve to facilitate exchanges (e.g., intermediary writings, seminars, etc.).



social sciences, and traditional ideas on the unity of science, since the 1970s these research projects have mainly concerned how to build and manage interdisciplinary projects, the practical and philosophical consequences of relationships between disciplines, the dynamics of interdisciplinary problem resolution, and the theory and methods of interdisciplinarity. The year 1972 is important in the history of interdisciplinarity, because of the publication of the OCDE book "Interdisciplinarity: Problems of Teaching and Research in Universities". Shortly after that, in 1979, two professional organizations were created: the Association for Integrative Studies (*AIS*) and the Association for the Study of Interdisciplinary Research (*INTERSTUDY*). These organizations structured the community of social science researchers who were working on the role of interdisciplinarity in the management of research, particularly by organizing conferences and publishing books. Furthermore, they offered a formal framework for collaboration between researchers, industry, and policy-makers (Thompson Klein, 1990).

The concept of a "discipline" is not static and can be defined in multiple ways. As Dominique Vinck (2000) clearly demonstrates, a discipline can be seen equally as a sociological entity (governed by a value system and rules that guide the behavior of its members); as a social network made up of links between researchers; as an epistemological and methodological framework (a body of concepts, methods, and intellectual postures); as an instrument of collective action (allowing the establishment of a hierarchy of topics, concepts, theories, methods, journals, laboratories, researchers) or as a tool that can be used by institutions that recognize and fund research.

Bruce et al. (2004, pp. 458) define disciplines as "stable systemic communities within which researchers concentrate their experience into a particular worldview". A discipline, then, would be an organizational category of scientific knowledge necessary for approaching the diversity of domains covered by science (Morin, 1994). The major benefit of organizing science into disciplines is that it facilitates the following: communication within the scientific community; a rigorous evaluation process; and legitimacy in the eyes of authorities outside science. The disadvantages of organization by discipline relate to the limits imposed on scientific inquiry and on the methods and the concepts that can be used (Bruce et al., 2004). The risk is of forgetting that the object of a research project is separated from reality based on the rules of the discipline and, therefore, is constructed by voluntarily ignoring certain features and links with other things (Morin, 1994). The consequence is that those elements related to an object of research that lie within a single discipline are

mistaken as being the complete and only realistic elements relevant to that object; a study that falls only within the bounds of a single discipline excludes all the characteristics and relationships that fall outside of that discipline. When this happens, problems naturally emerge in the interactions with other disciplines that study different aspects of the same reality by isolating a single object of research in a different way. Edgar Morin uses an evocative metaphor when referring to the proprietary mind of hyperspecialization: “We know that, originally, the word discipline was used for naming a small whip serving to self-flagellation, therefore allowing self criticism; in its inferior form, discipline becomes a way to flagellate the one adventuring in the field of ideas that the specialist consider to be his property” (Morin, 1994, p. 1).

Interdisciplinarity is close to, but distinct from, two other concepts: transdisciplinarity and pluri/multidisciplinarity (Mitchell, 2005; Grey and Connolly, 2008). The three concepts—interdisciplinarity, multidisciplinary, and transdisciplinarity—are not as much exceptions as they are the rule in the scientific community. Indeed, “if the official history of science is that of disciplinarity, another related and inseparable history is that of inter-trans-polydisciplinarity” (Morin, 1994, p. 2).

*Transdisciplinarity* is characterized more by the organization of knowledge into complex and heterogeneous domains or into transversal themes (e.g., order and chaos, structure and system, law and causality (Vinck, 2000)), than by an approach by discipline or subject. It supposes the construction of a new pattern of thinking, including concepts and methods that come from different disciplines but that are organized in a coherent framework (Mitchell, 2005). Edgar Morin (1994) gives the example of prehistory and the hominization process, which is simultaneously an anatomic, technical, ecological (savannah replacing the forest), genetic, ethological (behavioral), psychological, sociological, and religious phenomenon. In addition, the study of prehistory requires, for example, chemistry for dating prehistoric objects like bones and tools.

*Multidisciplinarity* addresses a single problem from the perspective of different disciplines, each of which maintains its structure, its function, its vocabulary, its patterns of evaluation, and the specificity of its academic community (Bruce et al., 2004, Grey and Connolly, 2008). Multidisciplinarity demands, therefore, a minimal collaboration between researchers and does not require a change in perspective. Even if information gathered via a multidisciplinary approach is richer than a single discipline approach, it simply juxtaposes contributions from distinct disciplines without producing results that can lead to a global understanding of the topic under study (Vinck, 2000). Multidisciplinarity

is the most common form of collaboration between disciplines, as it is the least disruptive of the existing practices. However, multidisciplinary does not necessarily lead to new approaches or to solutions to the real problems (an example would be the treatment of the same subject—let's say the loss of biodiversity—by two different disciplines, such as ecology and environmental economics).

Interdisciplinarity is more demanding, as it requires change and innovation in all aspects of research (structure, function, vocabulary, and evaluation patterns). Interdisciplinary research is based on conceptual models and methods that arise from different disciplines; the research perspectives change from one working stage to another, as needed (Aboelela et al., 2007). Interdisciplinarity assumes, therefore, a co-evolution of all disciplines concerned, issuing theoretical corpuses that will remain productive after the end of the project. Individual disciplines become richer from the process (Vinck, 2000). The field of ecology provides a highly relevant example of the way in which a new concept—that of the ecosystem—brought together knowledge from geology, chemistry, zoology, and botany—to create a new body of knowledge with its own internal coherence (Morin, 1994).

This brief overview of interdisciplinarity shows that it has benefited from numerous analyses; but, is an interdisciplinary approach relevant for addressing the current evolution of research practices in contemporary chemistry?

## **2. Does Contemporary Chemistry Need Interdisciplinarity?**

**LM:** Typically, one of two different motivations drives interdisciplinary research: the willingness to move a discipline forward, and the need to provide responses to pragmatic gaps in knowledge associated with real problems (Bruce et al., 2004). Each discipline contains knowledge within it that is related to how methods and tools are applied. Only practice provides a fine knowledge of advantages and disadvantages, as well as of the reach, significance, and interpretation of the results that arise from the use of these tools and methods. For this reason, interdisciplinarity is a vital necessity for certain projects that require knowledge about topics historically studied by other disciplines in order to progress (e.g., many studies in biology draw on principles of chemistry or physics) (Horwitz, 2003). For some areas of research, questions can be asked at several scales of time and space; these different scales are interdependent and interact. This makes it impossible to attempt to reduce the subject to a particular

disciplinary field. For example, a study of a marine ecosystem (Wind and de Kok, 2002) might need to simultaneously include a monthly analysis of the algal populations, a study of climate change on the scale of tens or hundreds of years, a study of human decisions regarding fishing or other issues on various scales, etc. In cases like this, interdisciplinarity is absolutely necessary to globally understand the research topic.

*Isabelle, does chemistry currently need interdisciplinarity?*

**IRL:** Of course, today more than ever. Chemistry is both a science and a major economic sector, at a global and at a national level. The chemical industry is indeed one of the key sectors of French industry, ranked second after the car industry and first among export sectors. France is Europe's second largest producer and its second largest exporter, after Germany.

However, chemistry is often viewed negatively by public opinion because of its association with pollution problems. Civil society and policy-makers have concerns about human health, environmental quality and, more generally, sustainable development that demand that the chemical industry and the academic research community engage in a radical revision to patterns of research, development, production, and use of chemical resources.

The European regulation REACH (Registration, Evaluation, Authorization and Restriction of Chemicals), in force since 2007, requires very precise data on the chemical properties, the toxicological effects, and the environmental impact of all molecules before they can be added to or retained on the market. This regulation completely modifies the vision and future of chemistry. It constitutes, indeed, an appeal to research to develop substitutes with more explicit and better-controlled health and environmental effects. This is also one of the questions raised during the "Grenelle de l'Environnement"<sup>3</sup>.

The major goal is to build strong and interdisciplinary academic research contributing to the development of chemistry that fully integrates the concept of sustainable development. This means economic development that is compatible with maintaining a healthy environment and an equitable social organization. This approach needs upstream acknowledgement of the need to "think and do chemistry differently"; to develop a green chemistry that respects the environment.

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<sup>3</sup> Grenelle de l'Environnement is a process launched in 2007 by the French Government for the participation of civil society in the development of a political roadmap in favor of sustainable development.

In the strategic plan of CNRS, called Horizon 2020, the main directions retained for academic research include finding solutions to global and complex problems related to the future of our planet (climate change, biodiversity, new energies, etc.), all by focusing the contribution of CNRS to the economic development of our societies. The responses to these challenges are necessarily interdisciplinary and collaborative. It is fundamental that CNRS integrate sustainable development into the research programmes; this was the reason why, in 2006, the Interdisciplinary Programme “Chemistry for Sustainable Development” (CPDD) was created. One of the main results from this programme is that a large number of research teams from CNRS and universities, as well as from organisms such as INRA (National Center for Agronomic Research), CEA (Center for Atomic Energy), CEMAGREF (Research Institute for Agricultural and Environmental Engineering), have already been identified and gathered together—about 900 researchers. The CPDD programme has been structured into four networks—each of which includes several working teams—that correspond to four major goals for interdisciplinarity in sustainable chemistry:

- 1—The use of renewable resources as raw materials and as the source of new products and materials.
- 2—Implementation of the principles of green chemistry (box 1) in new schemes of synthesis, including biotechnologies.
- 3—Optimization of environmentally friendly processes of chemical synthesis.
- 4—Evaluation and reduction of the impact of chemistry on the environment.

#### **Box 1**

##### **The twelve principles of green chemistry** (Anastas and Warner, 1998)

###### **1. Prevention**

It is better to prevent waste than to treat or clean up waste after it has been created.

###### **2. Atom Economy**

Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.

###### **3. Less Hazardous Chemical Synthesis**

Wherever practicable, synthetic methods should be designed to use and generate substances that possess little or no toxicity to human health and the environment.

**4. Designing Safer Chemicals**

Chemical products should be designed to effect their desired function while minimizing their toxicity.

**5. Safer Solvents and Auxiliaries**

The use of auxiliary substances (e.g., solvents, separation agents, etc.) should be made unnecessary wherever possible and innocuous when used.

**6. Design for Energy Efficiency**

Energy requirements of chemical processes should be recognized for their environmental and economic impacts and should be minimized. If possible, synthetic methods should be conducted at ambient temperature and pressure.

**7. Use of Renewable Feedstocks**

A raw material or feedstock should be renewable rather than depleting whenever technically and economically practicable.

**8. Reduce Derivatives**

Unnecessary derivatization (use of blocking groups, protection/ deprotection, temporary modification of physical/chemical processes) should be minimized or avoided if possible, because such steps require additional reagents and can generate waste.

**9. Catalysis**

Catalytic reagents (as selective as possible) are superior to stoichiometric reagents.

**10. Design for Degradation**

Chemical products should be designed so that at the end of their function they break down into innocuous degradation products and do not persist in the environment.

**11. Real-time analysis for Pollution Prevention**

Analytical methodologies need to be further developed to allow for real-time, in-process monitoring and control prior to the formation of hazardous substances.

**12. Inherently Safer Chemistry for Accident Prevention**

Substances and the form of a substance used in a chemical process should be chosen to minimize the potential for chemical accidents, including releases, explosions, and fires.

**LM:** *Several terms coexist today for naming this “new chemistry”, such as “green chemistry”, “sustainable chemistry”, “ecological chemistry”, “chemistry for sustainable development”, etc. What is the difference between these terms?*

**IRL:** First of all, “green chemistry” does not refer only to the “chemistry of renewable feedstock”, even if this is frequently how it is perceived. Green chemistry refers to the 12 principles developed by Paul Anastas. For me, “chemistry for sustainable development” or “sustainable chemistry” means something else. It is a larger term than green chemistry

that integrates the concerns for the economic viability of the result of the research.

Generally, research themes that fall within the field of sustainable chemistry include recycling and process intensification, and a closer link between catalysis and biocatalysis, chemistry and ecological engineering, etc. The most developed theme in France is the use of renewable feedstock. Beyond the confusion that has historically existed in France between “green chemistry” and “chemistry of renewable feedstock”, it is indeed the sector that has received most of the attention from industry and also from INRA. INRA has invested financial resources and has created research positions on this subject. Furthermore, France is an agricultural country; we have national potential for obtaining feedstock from agricultural products. The regions in France are starting to include renewable feedstock chemistry in their politics (in Midi-Pyrénées or Champagne-Ardenne for example, with competitiveness clusters<sup>4</sup> devoted to this issue). We can say that the state of research in France in this field differs from that in other European countries.

**LM:** The next section will address the details of interdisciplinary collaborations in sustainable chemistry, for understanding which disciplines are involved, why do they work together, and whether some of these common projects develop better than others.

### **3. Which Disciplines are Concerned with “Chemistry for Sustainable Development” and How do they Work Together?**

**LM:** Generally, the term “interdisciplinarity” refers to a synthesis between two or more disciplines, bodies of knowledge, or patterns of thinking, for producing explanations that are more powerful than each one alone could produce (Rhoten and Pfirman, 2007).

*Isabelle, which disciplines are concerned by each of the four networks of CPDD?*

**IRL:** The first network mainly involves biology, agronomy, and renewable feedstock chemistry. The second brings together domains of chemistry that did not work together before, such as catalysis, multi-stage synthesis, heterochemistry, etc., leading to a reconfiguration of the

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<sup>4</sup> Competitiveness clusters were first created in France in 2004, to facilitate closer collaborations between industry, research centers, and universities.

discipline through internal changes. The third network simultaneously engages chemistry and chemical engineering. The fourth brings together ecology, life sciences, and analytical chemistry.

**LM:** *Has involvement in this interdisciplinary programme significantly changed the research practices of the scientists involved? Or, is it more about making changes in the future as they continue their previous work? For example, did the disciplines you noted above work together before being involved in the CPDD?*

**IRL:** Some researchers were already involved in projects on sustainable chemistry before the CPDD, especially those working on replacing oil with renewable feedstock as a source of raw material for chemistry. Therefore, they were already working with life science experts from INRA, to understand the plant and its functional mechanisms. Other researchers were not used to working together, especially those involved in network 2, which is focused on chemistry, and in network 3, which is focused on processes. As well, network 4 links chemistry, ecotoxicology, and ecology. In this case, interdisciplinarity changed their practices. Indeed, the most important exchanges arose at the interface between chemical engineering and synthesis chemistry, and between chemistry and environmental sciences. For example, the interface between chemical engineering and synthesis chemistry deals with process intensification and implementation of synthesis micro-reactors. Another example, at the interface between chemistry and environmental sciences, is the association between chemistry and biotechnologies.

Of course, one cannot precisely quantify these changes in research practices at the interface with other disciplines. But through the CPDD they repeatedly interacted in a precise framework, and they had not done this before. They met during the three years of the programme; they directed PhDs together. Networking is an effective and low cost method for stimulating interdisciplinarity. It brings research communities together; they develop partnerships that can later produce larger projects, potentially funded by the National Research Agency (ANR<sup>5</sup>) or the European Commission.

It is also true that the interface between chemistry and toxicology and ecotoxicology is more difficult to establish than for other disciplines, simply because France is extremely short of toxicologists and ecotoxicologists. Since the 1980s, the State stopped its investment in these domains, both in

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<sup>5</sup> The National Research Agency (ANR) is the largest research funding authority in France. It funds both fundamental and applied research, proposed by teams coming from the public sector or collaborations between public and private research. URL: <http://www.agence-nationale-recherche.fr/en/about-us/missions/>



research and in universities, and we see the effects today. More so, since the implementation of the REACH regulation, which demands a significant number of (eco)toxicologists, given the high number of tests and risk assessments that need to be done. The research community is not ready to meet this demand, because of the scarcity of (eco)toxicology researchers and of the lack of relevant teaching programmes in universities.

**LM:** *This is paradoxical, because it seems to me that controversies and calls of NGOs and civil society that pertain to chemists mainly relate to the human health and environmental risks of a chemical; the assessment and mitigation of these risks relate directly to the domains of toxicology and ecotoxicology. Therefore, there is a real, societal demand for chemists to work more closely with these disciplines and to develop lower-risk or even “benign by design” substances, but interdisciplinarity has difficulties in answering this demand.*

**IRL:** Indeed. Implementation of the REACH regulation creates high demand for this type of competence. Available professionals are quickly absorbed by this new risk assessment market, to respond to the regulatory requirements imposed on the chemical industry. However, the lack of investment in toxicology and ecotoxicology in France continues—there are still few university training programs and research positions. Interdisciplinarity cannot develop over the long term, to work toward answering the practical questions, with insufficient disciplinary competence.

**LM:** *What might push chemists to work with toxicologists and ecotoxicologists?*

**IRL:** Beyond REACH, the nanotechnology debates that have taken place in France have stimulated chemists to think more deeply about the health risks associated with nanoparticles. Research funding institutions such as ANR also drive such collaborations. Finally, there is obvious social, political, and industrial concern about these issues.

**LM:** Even though interdisciplinary research has high sociopolitical importance and scientists are ready to work together, pragmatic factors seem to be key to really developing interdisciplinarity. The following section will address this issue.

#### **4. Are Financial Resources and Institutional Support Enough for Practicing Interdisciplinarity in “Chemistry for Sustainable Development”?**

**LM:** The literature shows that implementation of interdisciplinarity depends on the level of funding, on the incentives related to the scientific or industrial promotion of the results, on the institutional framework, and on the dynamics of the teams involved. The institutional context can significantly influence many factors, including the time available for each project, the management of the work of participating scientists, and the administrative control of the projects.

*Isabelle, who funds research on sustainable chemistry in France? Is the financial support adequate and correctly targeted towards interdisciplinarity?*

**IRL:** In sustainable chemistry, funding is currently relatively abundant. For example, the National Research Agency has a sustainable chemistry programme. The SusChem platform (European Technology Platform for Sustainable Chemistry<sup>6</sup>) also contributes, along with the Ministry of Industry via the Unique Interministerial Fund. At the European level, the field of sustainable chemistry has not been identified as such in the 7<sup>th</sup> Framework Programme (FP7) but it is present in several programs and will hopefully be present in FP8. Sustainable chemistry also exists within French competitiveness clusters such as Axelera in Lyon and IAR in Reims. Finally, there is funding from industry. Even though companies do not explicitly ask for sustainable solutions, we researchers propose sustainable chemistry solutions to industry’s practical questions.

However, the currently available funding is not balanced between the different themes of sustainable chemistry. For example, recycling—essentially an interdisciplinary theme—is currently poorly funded. A substance’s fate downstream from industry must be understood, depending on that substance’s uses. Furthermore, recovery methods must be found to restore the substance to its original quality and ensure its optimal reuse. Another, similar, example is energy. Chemistry can contribute both to recycling nuclear wastes and ameliorating photovoltaic power—the two domains are interdisciplinary, but which one gets funded is a political choice.

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<sup>6</sup> URL: <http://www.suschem.org/>

**LM:** *Does working on sustainable chemistry increase a laboratory's chance of getting funded?*

**IRL:** Yes, this is obvious. But, the dark side of the ease of finding funding for sustainable chemistry is that certain researchers use the term for getting grants without actually adhering to the principles of sustainable chemistry. We could call this “scientific greenwashing”. Even if a stage of the work is “greener”, this does not mean that a project is sustainable chemistry; sustainable chemistry is a continuum from development and production to the fate of a substance in the environment.

**LM:** *Does interdisciplinarity, which is necessary for sustainable chemistry, find enough institutional support in French research organizations and in universities?*

**IRL:** No, current support is not sufficient. Many chemists still do not see why they should take an interest in sustainable chemistry. They seem to be working under the illusion that sustainable chemistry is a question of fashion. At best, they “greenwash” their research to get grants; at worst, they are hostile towards this new way of thinking.

Chemistry for sustainable development demands a revision of the predominant way of thinking—currently oriented towards economy—to fully integrate ecological concerns. It also demands enough modesty to face the questions that citizens legitimately ask about the direction of “progress” or so-called progress. The recent events in Japan and the nuclear crisis at Fukushima demonstrate the fragility of our capitalist system, to which chemistry contributes. Presently, universities do not really contribute to awareness of these questions!

**LM:** Beyond the institutional and financial context of interdisciplinary research in sustainable chemistry, human problems related to collaborative work are equally important, as the following section reveals.

## **5. What Problems are Encountered by Teams Starting Interdisciplinary Work in Sustainable Chemistry?**

**LM:** Collaborative research is known to encounter several common problems. McCorcle (1982) highlighted two important differences between interdisciplinary teams and more homogenous and conventional teams.

1. The existence of the interdisciplinary team is driven by an exterior agent that can impose unexpected demands.
2. The diversity of members within an interdisciplinary team can be both a source of mutual enrichment and collaboration, and a source

of conflict. Exchanges within an interdisciplinary team reflect hierarchies exterior to that team, between the different disciplines involved. It has been shown that inside such a group, the status and roles of the members are defined depending on the existing hierarchy outside the group, in the absence of any other strong alternative. Even if such an alternative exists, the risk of breakdown is significant due to the diversity of career objectives, professional styles, and different ways of understanding and solving problems.

Several factors of interdisciplinary teams have been identified as those that contribute to a team's success (Thompson Klein, 1990): the number of people involved, the number of disciplines concerned, and the balance between the number of people representing each discipline. Among the aspects favoring interdisciplinary work, the team-building techniques used and the willingness to give time and effort to ensure efficient communication are very important (Bruce et al., 2004).

For example, Thompson Klein (2008) showed that the success of collaborative work largely depends on the willingness of researchers to learn from each other, on their ability to overcome disciplinary hierarchies (especially between "hard" and "soft" sciences), and on the reluctance of decisional structures of the research organizations to which researchers belong. Regarding the collaborative process, it is important to ensure that members of the interdisciplinary team are in frequent contact. If this condition is respected, group dynamics can facilitate the construction of a common identity, which must always be protected as it is fragile and temporary.

*Isabelle, have problems such as those described above arisen during the Interdisciplinary Programme that you manage? And if the answer is yes, how were they dealt with?*

**IRL:** The problems encountered are mostly related to the psychological difficulty that people have with moving off the beaten track. The networking I proposed was barely accepted by the CNRS management. However, networking is an excellent tool for developing interdisciplinarity. It allows research communities to get together, to discuss, and to know each other; interdisciplinarity then arises "naturally".

**LM:** Several techniques favor interdisciplinarity (Thompson Klein, 1990): regular meetings, common publications, common planning and objectives, internal and external seminars, mutual training, common data analysis, collective results and reports, mutual reviewing, common equipment, etc.

*Which were the tools used by the CPDD Programme to boost interdisciplinarity?*

**IRL:** We have used all of those above. The network structure functioned very well and we added seminars, common PhD supervision by two different disciplines, common publications, and common equipment.

**LM:** Researchers starting interdisciplinary work also require more time to become familiar with the subject. This can present some risks to the individual researcher and impose a disadvantage on his or her career, as the time required to become familiar with a new subject can slow a researcher's publication rate and his or her competence might be put into question by current research evaluation structures. Often, researchers go back to their original disciplinary approach once the interdisciplinary project is finished (Zanoni et al., 1998; Bruce et al., 2004).

*Is there a risk that the short duration (three years) of the Interdisciplinary programme "Chemistry for sustainable development" (CPDD) will end in scientists returning to their original discipline and their work before it?*

**IRL:** Indeed, time can be a problem. The interdisciplinary programmes of CNRS are often too short. I have tried to circumvent this by creating a Research Group. This is a tool available in the French research system that allows scientists to work together on the same subject for four to eight years.

At the same time, research teams have begun to form within laboratories, on subjects related to sustainable chemistry. The CPDD raised awareness within these laboratories, of the need to integrate sustainability concerns into chemical research. Of course, it is important to continue focusing funding on these themes because, currently, French laboratories direct their research according to the orientations given by the funding sources.

**LM:** Furthermore, interdisciplinary work for sustainable chemistry cannot last without appropriate promotion in researchers' careers and without explicit links to pragmatic questions that are important to industry.

## **6. Is Interdisciplinary Work in Sustainable Chemistry Promoted Correctly?**

**LM:** Between the 1970s and the 1980s, several publications described real situations in which scientists were involved in interdisciplinary

collaborations. This highlighted a paradoxical contradiction between the multiplication of discourses in favor of interdisciplinarity and the disadvantageous position that interdisciplinarity held in university curricula and research evaluation criteria, compared to disciplinary approaches (Thompson Klein, 1990).

It seems that, once disciplinary boundaries are overcome, the criteria for evaluating research cannot be the same as those for disciplinary work (e.g. agreement with the conceptual and methodological ground of the discipline, peer validation). This is especially true given that some benefits of interdisciplinary work cannot be measured, such as changes in attitude and research perspective among participants.

*Does engagement in interdisciplinary work and sustainable chemistry impact researchers' careers?*

**IRL:** Today, working on sustainable chemistry is more likely to favor a researcher's career, assuming that researcher does not lose his or her original disciplinary competence. In my team, for example, we work on sustainable chemistry but, in addition to this we work on organized systems—on supramolecular organization. We maintain expertise at the highest level of excellence on concepts of supramolecular chemistry and we are recognized for this double competence at an international level—both working on sustainable chemistry and on highly specialized disciplinary concepts. It is important not to be too generalist; not to lose one's distinctive value. This ability to be both very competent disciplinarily and flexible enough to address interdisciplinary questions demands a lot of effort, and it is an extremely difficult exercise. The researcher concerned has to attend different types of conferences. Furthermore, interdisciplinary work is time consuming, which can lead to fewer publications in the short term. This difficulty is not recognized in a researcher's career. When scientific work is evaluated, interdisciplinarity is not necessarily an advantage. It is not negative, but it is not an asset either. A similar situation also existed several years ago within the field of industrial promotion, which also demands work at the interface between fundamental and applied research. Currently, industrial collaborations are considered more favorably in research evaluation, but interdisciplinarity has not yet obtained the same recognition.

**LM:** *Is it easy to find a good journal for publishing interdisciplinary work in sustainable chemistry?*

**IRL:** Yes, this is not a problem in international journals related to this domain, if the work is good.

**LM:** Interdisciplinarity is characterized by a refusal of the dichotomy between research and action. Interdisciplinarity is seen as a way of reconstructing bridges between thinking and action, but opinions about the balance between the two diverge. Some believe that modern problems are so important that research and university teaching should be exclusively driven by the search for solutions. For others, it is only important that teams working on solutions to a problem receive more legitimacy in the academic community. Finally, for others, social problems are outside of the realm of research, which should be disciplinary and pure (Thompson Klein, 1990).

*Does interdisciplinarity in chemistry lead to the discovery of answers to concrete problems?*

**IRL:** Undoubtedly, yes. For this reason, sustainable chemistry is highly interesting from an industrial point of view. By its nature, interdisciplinarity is driven by concrete problems that cannot be solved using the theoretical resources of one discipline alone.

An example from my own experience is that of green galenics. Generally, galenics is the formulation of medicines, other therapeutics, or cosmetics. In my team, we have developed molecular economy and we apply it to medicines. From the beginning, products are developed that can formulate themselves, and in this way we develop a medicine that is both an excipient and an active substance. This is new and it is indeed a principle of sustainable chemistry that is applied to galenics. Using this technique, I already have two very competitive products on the market.

It is also true that not all the themes of sustainable chemistry are equally promoted in collaborations with industry. Today, markets do not favor those having virtuous practices in this field. It is easier for those industries close to the final user—the consumer—to demonstrate their engagement in green chemistry using marketing arguments. But other industries—those active, for example, during the intermediary stages of product development—have not yet found communication tools for informing consumers of their efforts.

**LM:** The richness of this experience you have, Isabelle, as manager of the Interdisciplinary Programme, Chemistry for Sustainable Development, incites me to go further by asking your feeling about should be done in French research in sustainable chemistry.

## 7. In Conclusion, What Would be the Actual Challenges of Interdisciplinary Research in Sustainable Chemistry?

**LM:** *Isabelle, what are the challenges for French research in sustainable chemistry?*

**IRL:** Undoubtedly, one of the main challenges is related to higher education. Indeed, students are not adequately aware of concepts related to sustainable chemistry. Teaching is still very disciplinary. However, if we agree that the challenges for innovation in sustainable chemistry depend on the fine balance between disciplinary developments and the ability to practice interdisciplinarity, it is important to teach both of these patterns of research practice to future chemists.

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As our dialogue shows, interdisciplinarity is not “natural”. It has to be learned and it has to be taught. While sustainable chemistry needs collaboration between chemists and their colleagues—ecologists, toxicologists and ecotoxicologists, biologists, agronomists, economists or sociologists—these experts are not always supported for starting and managing these interactions throughout their career.

Currently, a large body of literature exists that includes both case studies and theoretical and practical principles for orienting interdisciplinary work. Based on this literature and using a representative French case study, the present chapter brings some understanding about emerging research practices in chemistry, driven by interdisciplinarity, for answering social and political demands for better integration of sustainability concerns.

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# CONCEPTS OF EMERGENCE IN CHEMISTRY

ALEXANDRU MANAFU

## Introduction

Nowadays many philosophers of science would claim that reductionism as a philosophical programme has failed. The philosophical accounts of inter-theoretic reduction encountered theoretical and practical difficulties. It has been argued that examples of successful intertheoretic reductions in science are few and far between. As regards chemistry, many have expressed doubts that a reduction of this discipline to physics can be had.

On the other hand, nowadays almost everyone is a metaphysical naturalist. Chemists and philosophers alike contend that our world does not contain vitalistic chemical essences, spooky chemical souls, or chemical entelechies. They agree that if all the elementary entities that microphysics talks about (e.g., quarks, leptons, gauge bosons, fields, whatever) were to vanish, there would be nothing left: the atoms, the molecules and everything that is composed of them would also vanish. However, if all atoms and molecules were to disappear, the objects that form the subject matter of microphysics will not necessarily vanish; they may persist (e.g., as plasma). This asymmetry is a straightforward consequence of the direction of the composition relation: the objects that form the subject matter of chemistry are composed of the objects that form the subject matter of microphysics, but not vice versa. As a result, the latter may exist even in the absence of the former.<sup>1</sup> In this very narrow and precise sense then, the microphysical domain has ontological primacy over the chemical domain. This is sometimes referred to as “the generality of microphysics”—all events are, or are exclusively composed out of parts which are, microphysical events, and so fall under microphysical laws.<sup>2</sup>

It is hard to miss the apparent tension between the two claims made in the preceding paragraphs. If chemical stuff is composed of nothing else

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<sup>1</sup> Indeed, there was a time in the history of the universe when the objects that form the subject matter of chemistry did not exist.

<sup>2</sup> See for example P. Pettit (1993, p. 217).

except microphysical stuff, why doesn't chemistry reduce to microphysics? How could the chemical domain depend so strongly on the microphysical domain, yet not reduce to it?

A number of philosophers have provided reasons to think that the said tension is only *prima facie*. On their view, the generality of microphysics and the irreducibility of chemistry can be reconciled if we regard chemistry as emergent. According to the emergentists, all objects are composed—at their most fundamental level—of microphysical objects; however, it would be a mistake to conclude from here that all properties are physical properties; similarly, it would be a mistake to think that if all events are governed by physical laws then all laws must be physical. If emergentism is correct, there are genuine chemical properties and laws that do not reduce to physical properties and laws, although they are dependant upon them.

“Emergence” is a philosophical term of art, with a lot of appeal to philosophically inclined scientists, including chemists. However, the meaning of this term often remains underarticulated and vague. A prominent contemporary philosopher writes:

The term ‘emergence’ seems to have a special appeal for many people; it has an uplifting, expansive ring to it, unlike ‘reduction’ which sounds constrictive and overbearing. We now see the term being freely bandied about, especially by some scientists and science writers, with little visible regard for whether its use is underpinned by a consistent, tolerably unified, and shared meaning (Kim 2006, p. 547).

I don't think that the use of the term “emergence” is or should be reserved exclusively to philosophers. Also, I am quite sceptical that a unified meaning can be achieved for this term, even amongst philosophers. But I think there is a lot to learn if one pays attention to how philosophers—some of them with a chemistry background—have thought about emergence in chemistry. This paper reviews some of the most prominent concepts of emergence that have been offered so far in the philosophical literature about chemistry.

## 1. What is Emergence?

As Kim noticed, emergentist positions vary from one author to another and therefore emergentism is hard to pin down. However, there is a set of features that many emergentist positions share. Virtually all emergentist positions hold some form of the view that the world consists of a hierarchy of levels or ontological strata (the microphysical, the macrophysical, the

chemical, the biological, the psychological) and each level depends on the previous level, but it is irreducible to it. Properties at a certain level interact to produce properties at a higher level (emergents). The relation between the lower level and the higher level is usually thought to be supervenience: higher-level properties are said to supervene on the lower level properties.<sup>3</sup> These higher-level properties (emergents) arise from those at the lower level, but they cannot be predicted on the basis thereof. Emergents are often deemed to have novel causal powers, i.e., they have the capability to produce effects in a way that cannot be anticipated. Sometimes, emergents are said to be capable of downward causation—the ability to influence the basal conditions from which they arise (i.e., the underlying dynamics). Also, sometimes it is held that emergents involve global rather than merely local properties, and thus they arise only when the basal conditions are characterized by a certain amount of complexity. To sum up, emergents are usually characterized as novel, irreducible, unpredictable/unexplainable on the basis of the lower level theory, and on some views, capable of downward causation.

Typically, emergence is correlated with the failure of reduction. Depending on how one construes irreducibility, one ends up with different types of emergence. On the classical account of reduction due to Nagel (1961), one theory is irreducible to another if the laws of the higher-level theory cannot be deduced from those of a more fundamental theory by employing bridge laws connecting the two levels. For example, if there were chemical truths that cannot be predicted (deduced) from quantum mechanics together with the requisite bridge laws, one would say that chemistry is irreducible to quantum mechanics. However, the notion of predictability is ambiguous; it may refer to predictability in principle or to predictability in practice. If we hold a strong notion of predictability (i.e. predictability in principle) then we end up with strong emergence: chemistry cannot be reduced to quantum mechanics even in principle. If we hold a weaker notion of predictability (i.e., predictability in practice) then some weaker version of emergence obtains; in this case, we would say that chemistry is weakly emergent—chemistry cannot be *in practice* reduced to physics.

In chemistry, the following have been considered emergent or irreducible: chemical compounds, molecules, secondary properties of

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<sup>3</sup> A set of properties H supervenes on a set of properties L if and only if (i) any two objects x and y that have the same L properties will necessarily have the same H properties (though not necessarily vice versa), and (ii) any two objects z and w that differ in their H properties will also differ in their L properties (though not necessarily vice versa).

compounds such as their taste and colour, temperature, phases of matter, phase transitions, the shape of the molecules, atomic structure and properties, periodicity, aromaticity, chemical bond, chemical structure.

## 2. Early Accounts of Emergence in Chemistry

One of the earliest authors whose views about chemistry could be labelled as “emergent” is J.S. Mill (1806-1873). In *A System of Logic*, Mill talks about a *chemical mode* of causation, which he contrasts with a *mechanical mode*. In the mechanical mode of causation, the effect produced by two causes acting together is the sum of the effects of each cause acting independently. Mill calls this *the principle of composition of causes*, which in his view is akin to the principle of composition of forces in classical dynamics. On this mode of causation, the effect of the two causes acting in conjunction can be predicted deductively, from the effects of separate causes acting separately. The chemical mode of causation, on the other hand, does not obey the principle of composition of causes.

The chemical combination of two substances produces, as is well known, a third substance, with properties different from those of either of the two substances separately, or of both of them taken together. Not a trace of the properties of hydrogen or of oxygen is observable in those of their compound, water. (Mill 1882, p. 267)

In Mill’s view, chemical compounds have properties that are not “the sum” of the properties of their components taken separately or simply juxtaposed, as in a mixture. Besides the example of water, Mill gives the following examples: the sweet taste of sugar of lead (lead diacetate,  $\text{Pb}(\text{C}_2\text{H}_3\text{O}_2)_2$ ) is not the sum of the tastes of its component elements, acetic acid and lead or its oxide; the color of blue vitriol (copper sulfate,  $\text{CuSO}_4$ ) is not a mixture of the colors of sulfuric acid (transparent) and copper(II) oxide (black), from which it is produced. Those effects whose properties do not resemble the properties of their causes are called by Mill *heteropathic*; the laws governing the production of these effects are called *heteropathic laws*. For Mill, the laws of chemistry are heteropathic, since they govern the production of substances whose properties do not resemble those of the reagents.

It is unclear whether Mill’s conception of heteropathic laws is really at odds with reductionism. Admittedly, the properties of chemical compounds are not “the sum” of the properties of their components. But why should we expect them to be? A deductive explanation of the properties of chemical compounds in terms of the properties of their atomic constituents

could still be possible even if the manifest properties of these compounds are not “the sum” of the manifest properties of their components. Of course, for Mill such an explanation was out of sight. But as long as such an explanation remains possible in principle, Mill’s brand of emergentism would be classified as weak at best.

Charles Dunbar Broad (1925) also noted the distinction between purely mechanical behaviour and chemical behaviour. According to Broad, chemistry “seems to offer the most plausible example of emergent behaviour” (Broad 1925, p.65). For Broad, a system is emergent if its properties cannot be predicted from a knowledge of the properties of its constituents taken separately or in other wholes, and of their proportions and arrangements in this whole. According to Broad, the emergent properties of chemical compounds cannot be predicted from exhaustive knowledge of the properties of the parts—the only way to learn about them is to study samples of those compounds.

If the emergent theory of chemical compounds be true, a mathematical archangel, gifted with the further power of perceiving the microscopic structure of atoms as easily as we can perceive hay-stacks, could no more predict the behaviour of silver or of chlorine or the properties of silver chloride without having observed samples of those substances than we can at present. (Broad 1925, p. 71)

The same holds true about chemical affinity. According to Broad, we cannot predict that two elements would combine chemically with each other until we perform the reaction. One of Broad’s examples is that of hydrogen and oxygen:

Oxygen has certain properties and Hydrogen has certain other properties. They combine to form water, and the proportions in which they do this are fixed. Nothing that we know about Oxygen by itself or in its combinations with anything but Hydrogen would give us the least reason to suppose that it would combine with Hydrogen at all. Nothing that we know about Hydrogen by itself or in its combinations with anything but Oxygen would give us the least reason to expect that it would combine with Oxygen at all. And most of the chemical and physical properties of water have no known connexion, either quantitative or qualitative, with those of Oxygen and Hydrogen. (Broad 1925, p. 63)

It would seem that Broad’s view of chemistry fits squarely in what we called strong emergence: the properties of a chemical compound (including its ability to react with other chemicals) cannot be *in principle* predicted from the properties of the elements taken separately. According to Broad, this impossibility stems from the fact that the laws of chemistry

are “unique and ultimate” (Broad 1925, p. 65). By this, Broad means that they are not special cases which arises through substituting certain determinate values for variables in a general law which connects the properties of any chemical compound with those of its separate elements and with its structure. This, in turn, is due either to (i) the existence of innumerable “latent” properties in each element, each of which is manifested only in certain conditions, or (ii) to the lack of any general principle of composition, such as the parallelogram law in dynamics, by which the behaviour of any chemical compound could be deduced from its structure and from the behaviour of each of its elements in isolation (Broad 1925, p. 66-67).

Let’s consider the first possibility. According to a plausible interpretation of Broad, an emergent whole possesses force-generating properties of a sort not possessed by any of its parts (McLaughlin 2008, p. 41). When particles arrange themselves in certain configurations, new forces arise; these have been called *configurational forces*.<sup>4</sup> In chemistry, configurational forces are higher-level chemical forces characterizing the compounds, irreducible to lower-level physical forces characterizing the components. They are responsible for the existence of emergent behaviour (chemical affinity, the properties of the compounds). Configurational forces are contrasted with *resultant forces*, i.e., non-emergent forces that are the generated by other forces, not by configurations of particles; “emergence”, therefore, is contrasted with “resultance”.

If the second possibility obtains, one cannot learn about the properties of a compound by substituting certain values of the variables in a general law which connects the properties of that compound with those of its constituents, for there is no such general law. This would explain why the trans-ordinal laws that connect the properties of the atoms with those of compounds are *unique* and *ultimate*. They are *ultimate* because in determining the properties of a chemical compound there is no theoretical shortcut, one must study a sample. They are *unique* because by studying the rule Nature follows when it produces a certain compound one cannot learn anything about the rule Nature follows when it produces other compounds.

Is Broad’s emergentism weak or strong? Given Broad’s “mathematical archangel” metaphor, one would think that Broad’s emergentism is of the strong kind. But caution is required if we try to establish whether or not on

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<sup>4</sup> Although Broad does not use this term, McLaughlin (2008) interprets Broad in this way. According to McLaughlin, “it is clear that he [i.e., Broad] maintains that certain structures of chemical compounds can influence motion in fundamental ways” (McLaughlin, 2008, p. 47).

Broad's view chemistry is strongly emergent. Broad was aware of the possibility that the laws of chemical combination and the properties of compounds could turn out to be mere consequences of the laws of microphysics (Broad 1925, p. 73). Indeed, it has been argued that the advancements in the understanding of the atomic and molecular structure that took place during the 20<sup>th</sup> century make Broad's claims regarding emergence in chemistry implausible (McLaughlin 2008). If these arguments are sound, Broad's emergentism may be strong, but chemistry is not an example of strong emergence.

### 3. Contemporary Accounts

A recent approach to emergence in chemistry is due to Hendry (2006). Hendry's account is based on the classical notion of emergence advocated by Broad. Hendry does not accept McLaughlin's conclusion that there is no scintilla of evidence that there are configurational forces or downward causation in chemistry; he adopts McLaughlin's distinction between resultant and configurational but he formulates it in terms of Hamiltonians, rather than forces. Using the quantum chemistry of the molecule, Hendry aims to show that there is downward causation in chemistry by showing that there are "configurational Hamiltonians" governing the behaviour of molecules.

Hendry asserts that if the behaviour of some systems is governed by configurational (non-resultant) Hamiltonians, then the behaviour of those composite systems is not determined by the more general laws governing their constituents. He argues that to the extent that the behaviour of any subsystem is affected by the supersystems in which it participates, the emergent behaviour of complex systems must be viewed as determining, but not being fully determined by, the behaviour of their constituent parts. This, Hendry contends, is the case in the physical chemistry of the molecule, where the motions of the atoms are determined by the overall structure of the molecule.

Hendry uses the concrete example of a CO<sub>2</sub> molecule. The parts of this molecule can be seen as quantum mechanical harmonic oscillators and rigid rotators. However, this is possible only after we assume a certain structure for the whole molecule. Hendry points out that we use quantum mechanics to explain the motions of parts of the molecule within the context of a given structure for the molecule as a whole (in this case, a linear structure). The problem is that rather than deriving this structure using resultant Hamiltonians, we put it "by hand"—we assume "configurational Hamiltonians". The fact that the motion of the parts of



molecule is determined by the overall structure is, according to Hendry, an example of downward causation.

Is the chemical emergence that Hendry's arguments support of a strong kind? If the molecular Hamiltonians are truly configurational and thus fundamental (i.e., not resultant), then the kind of emergence that Hendry's arguments support is strong. If, however, they are resultant, then Hendry's arguments support only weak emergence. The advocate of weak emergence may agree that the molecule as a whole constrains (determines) the motion of its parts. But she may argue that its ability to do so comes from the intrinsic and relational properties of the parts themselves (from the Coulomb attractive and repulsive forces between the parts and various other factors such as the Pauli principle, relativistic effects and even gravity). On this view, the use of configurational Hamiltonians is justified for pragmatic reasons (resultant Hamiltonians are just too hard to compute) or epistemic reasons (having to do with their explanatory role), but from an ontological perspective these Hamiltonians are ultimately resultant, albeit often unobtainable in practice. Nonetheless, Hendry's own view seems to be that the molecular Hamiltonians are not resultant, so he seems to regard chemistry as strongly emergent.

Hendry claims that his revision of traditional emergentism is at odds with the causal completeness (or causal closure) of physics—the thesis that “all physical events are determined (or have their chances determined) entirely by prior physical events according to physical laws” (Papineau 1990, p. 67). If chemistry truly denies the causal completeness of physics then it would seem that this constitutes evidence for a strong notion of emergence; presumably, the existence of non-physical but causally efficient properties (such as *sui generis* chemical properties) guarantees that what's true about them cannot be derived from the truths of microphysics. If one thinks that the causal closure of physics is grounded in the conservation of energy, it is not entirely clear how a strong version of emergence that denies it may respect this venerable principle of science.

Another recent approach to emergence in chemistry is due to Paul Humphreys (1996; 1997a; 1997b). Humphreys' account is original because it denies that the relationship between higher-level emergent properties and lower level properties is supervenience (1997a). Instead, it links emergence with the existence of a fusion operation that operates on *i*-level properties and outputs *i*+1-level properties, which have novel causal powers.

Humphreys' fusion process is formally represented as follows. Let  $P_m^i(x_r^i)t_1$  represent an *i*-level entity,  $x_r$ , instantiating an *i*-level property,  $P_m$ , at time  $t_1$ .  $P_n^i(x_s^i)t_1$  will denote another *i*-level entity,  $x_s$ , instantiating

another  $i$ -level property,  $P_n$ , at time  $t_1$ . Humphreys introduces the *fusion operation* symbolized by  $[*]$ , which takes as arguments the two property instances  $P_m^i(x_r^i)t_1$  and  $P_n^i(x_s^i)t_1$  and fuses them:  $[P_m^i(x_r^i)t_1 * P_n^i(x_s^i)t_1]$ . The fusion operation is an  $i$ -level operation, i.e., an operation of the same level as its arguments. The result of the fusion operation is the fused property  $[P_m^i * P_n^i](x_r^i * x_s^i)t_2$  at the  $i+1$ -level, which can also be written as  $[P_m^{i+1} * P_n^{i+1}](x_r^{i+1} * x_s^{i+1})t_2$ . This property is what is emergent on Humphreys' account. The fused property is a unified whole in the sense that its causal effects cannot be represented in terms of the separate causal effects of the original property instances.

According to Humphreys, the non-separable states of quantum mechanics are examples of fusion emergence. A composite non-separable quantum system is holistic, in that the joint system possesses a state while the components taken individually do not. Given that quantum entanglement has a role in chemical bonding (via the Pauli Exclusion Principle), one would be tempted to claim that molecules are an example of fusion emergence.<sup>5</sup>

Humphreys' account of emergence was motivated by the desire to avoid the threats of the exclusion argument for reductionism, which states that higher-level emergent properties are excluded from affecting lower-level properties, since all the causal work is done by the latter (see Kim 1992; 1999; 2006). Humphreys argues that at the time when the fused property instance  $[P_m^i(x_r^i)t_1 * P_n^i(x_s^i)t_1]$  comes into existence, the original property instances  $P_m^i(x_r^i)t_1$  and  $P_n^i(x_s^i)t_1$  cease to exist. Therefore, it is *a fortiori* the case that they cannot compete as causes with the emergent property instance. On Humphreys account, emergents don't coexist with their bases, and this feature prevents the exclusion argument to get off the ground.

Humphreys explicitly suggests that his version of emergence challenges the assumption that the physical domain is causally closed (Humphreys 1997b, p. 3). The causal closure thesis asserts that the ultimate causes of all physical effects are themselves physical and is often taken to be

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<sup>5</sup> See Humphrey's conference talk titled "A defence of ontological emergence" which was presented at the International School on Complexity 9: Emergence in the Physical and Biological Worlds, Ettore Majorana Foundation, Sicily, in 2008. Since Humphreys has not turned this conference paper into a publication (yet), it is uncertain whether he is still committed to the view that molecules exemplify fusion emergence.

synonymous with the completeness thesis. Just as Hendry's emergentism, Humphreys' fusion emergence seems to be of a strong kind. Given that on Humphreys' account (some of) the properties of the parts are used up in the process of the formation of the whole, it would seem that a (synchronous) derivation of the properties of the whole from the properties of the parts is precluded in principle; this would further support the idea that fusion emergence is strong (synchronous) emergence.<sup>6</sup>

A number of contemporary authors have recently proposed concepts of emergence that are applicable to phenomena studied by science in general. Although the examples that these authors refer to come from specific domains (the theory of cellular automata, physics, etc) these concepts of emergence are applicable to a host of phenomena, including those in the purview of chemistry.

Mark Bedau (2008) thinks that there is not much room for strong emergence in contemporary science, and even if such strongly emergent phenomena existed, they could at best play a primitive role and thus they will be scientifically irrelevant. Bedau defends a version of emergence that he even refers to as "weak emergence". Weak emergence is compatible with the generality of microphysics:

Macro entities and their states are wholly constituted by the states and locations of their constituent micro entities, so the causal dynamics involving macro objects is wholly determined by the underlying micro dynamics. (Bedau 2008, p. 161).

But Bedau also recognizes that the global properties of a macro system may influence the behaviour at the micro-level. This is a sort of downward causation; however, the kind of downward causation is not the same as the fundamental kind of downward causation that is associated with strong emergence. The properties of the macro system (including the causal properties) are a consequence of the properties of the micro systems that compose it, but the derivation is usually hard to obtain. The hallmark of Bedau's weak emergence is that to obtain such a derivation there is no theoretical shortcut: one must resort to simulation. Bedau claims that causal processes in nature are caused by the iteration and aggregation of

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<sup>6</sup> This leaves open the possibility that what counts as strong emergence from the synchronous perspective would qualify as weak emergence if a diachronic notion of derivability is favoured. Besides these temporal aspects, the issue of whether Humphreys' fusion emergence is strong or weak is further complicated by various factors such as the nature of the fusion process and the potential differences between completeness and causal closure. This is not the place to address all these complications.

micro causal interactions. The only way to predict the macro properties of weakly emergent systems is to follow the same steps of iteration and aggregation that Nature follows, with the help of powerful computers.

Bedau's examples of weak emergence come primarily from the theory of cellular automata. For example, being a glider gun is a weakly emergent property in the Game of Life—a glider gun is a macro-level property, which is realized by a variety of micro-level configurations of cells. Thus, Bedau's emergence is compatible with a weak notion of reductionism—*token* reductionism, which claims that all property instances are lower level property instances; but insofar it is committed to the idea that the same macro property can be instantiated by a variety of different micro properties (see the multiple realizability of the glider gun example), Bedau's emergence is incompatible with *type* reductionism—the idea that all properties are lower level properties. According to Bedau, explanations that contain emergents (macro explanations) are autonomous in relation to micro explanations—they are overarching explanations that unify an otherwise heterogeneous collection of micro instances.

Concepts of emergence that emphasize context sensitivity, nonlinearity, feedback loops, and the importance of organization between the parts of compositionally complex systems have been presented by William Wimsatt (2000; 2008) and Sandra Mitchell (2010). These accounts of emergence are not intended to apply to chemistry in particular and they seem to be compatible even with a strong notion of reduction (type reductionism). This is why those inclined to see reductionism (or at least a strong variant thereof) and emergence as mutually exclusive would not readily embrace these accounts as emergentist. Indeed, what these accounts call “emergence” would actually count as “resultance” in the eyes of those who hold more conservative views about emergence.<sup>7</sup>

An emergentist account intended to apply to specifically to chemistry has been offered by Luisi (2002). By the term emergence Luisi understands the onset of novel properties that arise when a certain level of structural complexity is formed from components of lower complexity. Luisi emphasizes that molecular sciences, and chemistry in particular, are actually the disciplines in which the notion of emergence has the most obvious applicability. Luisi offers the following examples of emergent properties in chemistry: the aromaticity of a benzene molecule, which is not present in the atoms that form the molecule; the properties of water and of all other molecules, which are not present in the atomic components;

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<sup>7</sup> For a discussion of the distinction between emergence and resultance in the context of British emergentism, see McLaughlin (2008).

and the oxygen-binding properties of complex chemical structures like hemoglobin or myoglobin which are not present in the single aminoacids.

Luisi considers the following two questions. Can the properties of molecules be explained *a posteriori* from the properties of the components? Can they be foreseen *a priori*? Luisi argues that there are no reasons to think that the liquid properties of water, the aromaticity of benzene, or the folding of myoglobin, cannot be in principle explained or even foreseen on the basis of the properties of the components. Thus, Luisi seems to be entirely committed to token reductionism. He even goes as far as claiming that the hypothesis that the emergent properties of molecules cannot be explained as a matter of principle on the basis of the components is tantamount to assuming a force of some non-defined nature (Luisi 2002, p. 193).<sup>8</sup> But he points out that in practice, emergent properties are almost impossible to predict. This is especially true for large molecules like myoglobin, in the case of which the 20 different amino acids and a chain length of 153 amino acid residues, gives rise to  $20^{153}$  possible theoretical chains, myoglobin being one of those.

According to Luisi, chemistry offers examples of downward causation, understood as the influence of the relatedness of the parts on the behaviour of the parts themselves. One example that Luisi offers is that of benzene: when a benzene molecule is created, the orbitals of carbon atoms and those of hydrogen are changed; the molecule as a whole affects the properties of its constituents. Of course, it is true that the molecule of benzene could not have emerged if its components did not have the right properties (Luisi does not deny upward causation), but it is also true that once the molecule is formed it constraints the motion of its parts. For Luisi, downward causation is the consequence of upward causation, and once the two exist, they take place simultaneously in a sort of “cyclic” causality. But the kind of downward causation that Luisi endorses differs significantly from the kind of downward causation that the British emergentists talked about; it does not assume any special forces at work other than the normal laws of physics.

Luisi's account of emergence resembles very much Bedau's weak emergence, especially when one compares the two authors' views about predictability and downward causation.

Another concept of emergence has been offered by Robert Batterman (2002; 2010). Although Batterman's examples of emergence are primarily

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<sup>8</sup> It is plausible to think of this force of a non-defined nature that Luisi talks about as a “configurational force” in McLaughlin's terms.

from physics, his view of emergence has the potential of applying to chemistry as well, and for this reason it is worth mentioning.<sup>9</sup>

Batterman distinguishes between two senses of reduction. One may talk of the reduction of one theory to another in the philosopher's sense (e.g., Nagelian reduction, where the laws of a coarse grained theory are derived from the laws of another, fine-grained, theory); or one may talk of reduction in the physicist's sense (the fine grained theory reduces to the coarse grained theory in the limit of some parameter having a certain value). For example, relativistic mechanics reduces to classical mechanics in the limit in which  $(v/c)^2 \rightarrow 0$ . Now, the limiting relations between theories may be *regular* (when the "limiting behaviour" as the parameter tends to a certain value resembles the "behaviour in the limit", where the parameter has that value), or they may be *singular* (when the behaviour in the limit differs markedly from the limiting behaviour). Many pairs of theories are related by singular limiting behaviour: quantum and classical mechanics, the wave and ray optics, statistical mechanics and thermodynamics.

For Batterman, the singular nature of the limiting relations between pairs of theories is indicative of emergence: the behaviour of the system as certain parameter approaches a certain value is different from the behaviour of the system when that value is reached. When the limiting relations are singular we can expect novel phenomena in the asymptotic regime between the two theories. Often, such in the case of thermodynamics and statistical mechanics, the coarser (higher level) theory can be derived (reduced in the philosopher's sense) from the fine grained (lower level) theory only if one makes the assumption that when a certain parameter (viz. the number of particles,  $N$ ) approaches infinity. But real systems are always finite, and a strict derivation obtains only in the thermodynamic limit. As a result, one may speak of the phenomena of thermodynamics as emerging from statistical mechanics. Qualitative changes in the states of matter known as phase transitions (e.g., freezing and boiling water, the transition from the ferromagnetic phase to the paramagnetic phase) are also considered emergent since it proves very difficult (if not impossible) to reduce them to the underlying microphysics if we do not appeal to infinite idealizations.

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<sup>9</sup> In fact, if one regards thermodynamics and statistical mechanics as disciplines that equally fall within the purview of chemistry (as many chemistry textbooks do), Batterman's notion of emergence is applicable to at least this chemical example.

Batterman's approach pays close attention to mathematical procedures such as renormalization—a mathematical technique for characterizing how the structure of interactions varies with the scale considered. Renormalization reveals how theories at different levels are related, but such relation is not reduction: it turns out that the phenomena studied by the higher-level theory are decoupled from those at the lower level.

For Batterman, emergence is also associated with universality or multiple realizability (systems very different at the micro-level exhibiting identical macro-level behaviour). Multiple realizability shows that lower-level explanations cannot adequately account for the convergence of the behaviour of varied systems, and higher-level level explanations that ignore the micro-level details are required. In contrast with the classical notions of emergence, Batterman's notion of emergence does not subscribe to the downward causation thesis or to the idea that mereological part/whole relations play a crucial role in emergence.

There is another concept of emergence that applies to chemistry, but so far both chemists and philosophers of chemistry have not acknowledged it—I'll label it "functional emergence". Functional emergence refers to the idea that many chemical properties are defined not by a shared microphysical ingredient, but functionally, by a common behaviour. Take, for example, the property of being an acid.<sup>10</sup> The property of being an acid is defined functionally, by pointing to a common behaviour of these substances in chemical reactions (the ability to donate a proton, on the Brønsted-Lowry theory) rather than to a shared microphysical ingredient (a hydrogen atom, for example).

Functional emergence is committed to the generality of microphysics: e.g., every acidic molecule is a complex microphysical system of interacting electrons, protons and neutrons, all obeying the laws of physics (token reductionism is respected). However, functional emergence agrees that it would be mistake to conclude from here that chemical properties are microphysical properties in disguise.<sup>11</sup> Similarly, it rejects the idea that if all events are governed by physical laws, then all laws must be physical. According to functional emergence, there are genuine chemical properties and laws, which are type-irreducible to the properties and laws of microphysics. The reason for this is multiple realizability: one and the same chemical property (e.g., acidity) is realized by a variety of

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<sup>10</sup> Many other examples of chemical functional properties can be given: being a base, an oxidant, a reductant, a metal, or being a piezoelectric.

<sup>11</sup> A chemical property is a physical property in disguise if the chemical property is identical with a very complex physical property but this identity relation is not obvious.

microphysical lower level properties (systems of electrons, protons and neutrons), and thus it cannot be identified with any particular microphysical constitutive property. As a result, the laws in which functional chemical properties occur will not be derivable from the laws of microphysics simply because the latter lack the requisite terms. Since derivability seems to be impossible in principle, functional emergence seems to qualify partially as strong emergence. I say partially because only the chemical laws that contain terms denoting functional properties cannot be derived, but particular chemical events may still be predictable from the underlying physics. However, unlike other varieties of strong emergence, functional emergence does not go as far as to deny the causal closure of physics.

## Conclusion

Developing accounts of emergence in chemistry is important because emergence typically offers a way of reconciling the failure of reduction with the commitment to the generality of microphysics. In addition, emergence seems a promising way to secure the ontological autonomy of chemistry. If a theory of chemical emergence can demonstrate that chemical properties are not just complicated microphysical properties in disguise, then chemistry is autonomous from microphysics not only from a historical, epistemic or pragmatic point of view, which is never contested, but also from an ontological one, which is more problematic.

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# DOWNWARD CAUSATION WITHOUT FOUNDATIONS

MICHEL BITBOL

## Introduction

Downward causation looks impossible as a concept, but is well established as a fact. A top-down flux of causation going from an emergent level of processes (say biological or mental) to the fundamental level of processes (say physical) that is supposed to *underpin* it, sounds like a paradox. Yet this paradox seems to be forced upon us when we want to make sense of many phenomena ranging from psychosomatics to the mutual interaction between organismic and cellular life, for instance when we want to express certain facts of experience in which a change in our mental state has an immediate impact on our physiological state. My conviction is that what is likely to be paradoxical here is neither experience nor even its verbal expression in terms of downward causation, but the standard *metaphysical interpretations* that are superimposed onto them.

The metaphysical conception to be dispelled when downward causation is at stake is a *dualist* and *foundationalist* picture: a picture according to which downward causation only makes sense if there are at least *two* (ontologically) distinct levels of processes, with their own specific entities and properties able to influence each other by way of efficient causality. This is also a picture in which, conversely, if there *exists* only *one* fundamental level of being and process, then the very concept of inter-level causation is pointless. To counterweight this popular picture, I will advocate in this article the idea that the phrases ‘downward causation’ and ‘upward causation’ are loose ways of describing two modalities of *action* exerted on a process, which nothing prevents one from construing as non-dual. Acting globally (or coarsely, at a large scale) yields consequences that can be detected by experiments bearing on local levels. Conversely, intervening at the smallest accessible scale yields

consequences that can be detected by experiments bearing on the larger scale. On the basis of this account, I will conclude that:

- (i) Downward and upward causation are *neither* illusory *nor* inherently existent, but rather *indexed* by a certain level of intervention. Accordingly, downward and upward causation are not substantial concepts, but rather relational concepts throughout.
- (ii) The relevant relations do not take place between otherwise self-subsistent entities. They contribute to the very *definition* of their terms. These defining relations are primarily the relations between the agents and the targets of their actions; and secondarily the relations between various domains of acting and experimenting.

Point (i) amounts to replacing ontological dualism with functional duality of domains of intervention. As for point (ii), it dispels foundationalism from the outset. Instead of the usual scheme of intrinsically “basic” and “emergent” levels of being (or levels of organization), one is left with flexible levels of (experiential and experimental) access, levels of action, levels of analysis, and levels of theorization.

This strongly anti-foundationalist approach does not fit well with the dominant scientific realist program of research in philosophy of science. But it makes perfectly good sense in the framework of an alternative program of research<sup>1</sup> inspired by Kant’s “transcendental idealism,” Husserl’s phenomenology, and pragmatism. After all, in this kind of framework, “the access to an object partakes of the being of this object” (Levinas 2001, 161).

## 1. Paradoxes and Difficulties of Downward Causation

The central difficulty, expressed by Jaegwon Kim (1999), is the threat of vicious circularity. Is it coherent, Kim asks, to assume that the presence of a certain lower-level process is “responsible” for the presence of a higher-level process, and yet the higher-level process somehow exercises a causal influence on the lower-level process? Since the higher level entirely arises from the lower level, the idea of downward causation sounds either contradictory or redundant. It contradicts the rest of science if it really makes a difference, by violating the micro-laws that rule the

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<sup>1</sup> For applications of this research program to the philosophy of quantum mechanics, see M. Bitbol (1997, 1998, 2000, and 2001). A former version of this research has been published in *Synthese*, 233-255, 2012.

low-level. And it is redundant if it merely restates in a different language, a coarse-grained language, what could, at least in principle, be couched in the fine-grained language of the detailed micro-processes.

Let us dig a little deeper below the surface of the two latter sharp statements. The first statement is meant to dismiss the idea of strong emergence, according to which the high-level processes are endowed with autonomous causal powers, and with ability to alter the low-level processes. It does so by assuming that for high-level processes to count as causal powers in the fullest sense, and to be able to alter anything significant in the lower level, they must induce a deviation in the *laws* of the micro-processes. But if this were the case, two common presuppositions of the scientific picture of the world would be denied: (a) the presupposition of nomological closure of the lower micro-*physical* level, and (b) the presupposition of *causal fundamentalism*, according to which “macro causal powers supervene on and are determined by micro causal powers” (Bedau 2002, 10). Strong emergence thus apparently amounts to an indefensible variety of ontological dualism.

Now, what about the second statement, which explores the other end of the spectrum of positions about emergence? It says that if the higher level makes no real difference, to wit (in this framework of thought) if no alteration of the micro-laws is imposed by it, then the very concept of a high level and of its causal powers is of no other significance than purely *verbal*. Instead of strong emergence, we are left with *nominal* emergence, and instead of dualism, the flattest possible version of monism: reductionism.

Kim’s line of argument thus leads us towards an unacceptable alternative: either ontological dualism or ontological monism with epiphenomenalism.

Before I address these central difficulties, I wish to deepen the crisis of downward causation by three additional remarks.

(1) Since *efficient* causality seems to be at stake, one is inclined to examine the consequences of one of the most popular conceptions of the cause-effect relationship. This conception states that for a causal relation to arise, there must be a *transfer* of some conserved quantity (say *energy*), from the cause to the effect (Salmon 1984). Here, “transfer” must be taken literally as: (a) loss of energy on the one side, and (b) gain of energy on the other side. But this immediately strikes us as problematic when upward and downward causation are concerned, if one embeds them within the framework of elementary physics interpreted with substantialist presuppositions. For, if this framework is upheld uncompromisingly, a

pattern of organization can hardly be said to carry energy *by itself*, but only *qua* being made of interacting material constituents. This being granted, energy can be transferred from one material object to another object (by way of mediators), but not from a set of material constituents to their own global organization abstracted from what it organizes.

(2) According to the same conception, causal relations necessarily involve succession in time. Cases of simultaneous causation are shown to be only *apparent*, since, in view of a basic postulate of special relativity, they involve a quick but not instantaneous transfer of information and energy (Kistler 1999, 57). Now, it is quite clear that, between an emergent level of organization and its alleged physical basis, there is no time-lag (except if one considers the progressive rise of the higher level in history, or the possibility of predicting it (Stephan 1998)). Claiming that a set of interacting molecules *first* causes the biological organism to arise (upward causation), and that this biological organism *then* causes its own pattern of chemical reactions to adopt such and such configuration (downward causation), is an artifact of our discursive and sequential language. It would be more appropriate to claim that the basic elements *make up* the higher level of organization, *at the same time* as the higher level of organization *defines* the boundaries of the constituting interactions between the basic elements (Emmeche et al. 2000). “Making up” and “defining boundaries” are simultaneous, unlike causal relations.

(3) The standard idea of emergence is that a certain *form, pattern, “topology”* or “configuration” (Deacon 2003) supervenes on a basis made of the intrinsic properties of the components. This model is borrowed from classical physics. For instance, in classical electrodynamics, the interaction between N particles (as well as the configuration that arises from it) is supervenient on their electric charges and their positions. Within this configurational view of emergence, a dual picture of the various levels is automatically generated. The lower level is made of substances and properties, whereas the higher level is made of pure patterns. Such a duality triggers questions about a possible influence of one layer on the other, but the answer to those questions is preempted. Indeed, “upward causation” here holds only in the trivial sense of a set of properties determining their network of interactions. As for downward causation, it is made implausible by the difference in ontological status of the two levels. Figuring out how a configuration may act *as such* on a layer of basic properties is quite problematic. It would be more acceptable, in the spirit of the substantialist construal of the basic level, to say that the

properties of the constituents cooperate to circumscribe their own range of possible variations, than to claim that their global configuration *causes* their alteration. But in this latter case, no motive for supposing a duality of levels is left; speaking in terms of mutual causation between these levels becomes pointless.

At this point, one realizes that, in a framework of thought that associates a substantialist conception of the basic level and a configurational conception of the emergent levels, talk of upward or downward causation is at the same time *irresistible* and reduced to the status of a *purely verbal machinery*.

## 2. Partial Solutions: The Inheritance of Aristotle and Kant

Several ideas have been offered to solve some of these difficulties, while sticking (implicitly or explicitly) to the substantialist view of the basic level. But, as we will see, they are not sufficient to account for the types of experiences and experiments that give support to the concept of downward causation.

The common ground of these ideas consists in using alternative concepts of causality, borrowed from Aristotle's well-known tetrad. The motivation for this attempt is that the formerly listed difficulties are connected with some typical features of the concept of efficient causality. So why not make use of formal causality, material causality, and even final causality?

It is quite natural, in the standard framework of thought, to consider that the basic constituent elements are the *material causes* of the emergent levels of organization, whereas, conversely, these emergent levels act as *formal causes* which circumscribe a domain of variation for the properties of their elements. Upward causation then instantiates the species of *material causality*, and downward causation initiates the species of *formal causality*. The former concepts of "making up" and "defining boundaries" are thereby encompassed within a broad class of causal connections (Varela 1976), in spite of their being foreign to *efficient* causality.

The concept of formal causation can be developed by borrowing concepts from dynamics: The concept of *boundary conditions* and the concept of an *attractor*. The higher level of organization of a process can be described as a self-imposed *boundary condition*. Among all the possible solutions of the differential equations describing the dynamics of the parts, such a boundary condition selects a range of *accessible* solutions. This substantiates the idea that the higher level *constrains* the

evolution of the constituent elements, at the same time as it is *made up* by them. Alternatively, the higher level of organization can be characterized as a global *attractor* for the trajectories of the constituent elements in phase space. This attractor *shapes out* the evolution of the elements at the same time as it is *determined by* their states and interactions (Emmeche 2000).

The fourth and last species of causality shows up at this point. A two-way process of making up and constraining, within an integrated unit called an “organism,” gives rise to the *appearance* of what Kant called “natural purpose” in his *Critique of Judgment* (§64-66). According to Kant, in order for something to be construed as a natural purpose, a crucial condition is that “(...) the parts of the thing combine into the unity of the whole because they are *reciprocally cause and effect of their form*” (Kant 1987, 252). Such an integrated process can indeed conveniently be thought of as produced by a *final* cause, insofar as everything in it occurs *as if* the very *concept of the organism* as a whole were the cause of the distribution of its parts.

In another paragraph, Kant characterizes this reciprocity of action between the parts and whole by using a vocabulary that is strikingly close to the current one, yet virtually reverted (Kant 1987, 251). In Kant’s terms, a “descending series” is a chain of determination of effects by efficient causes. And an “ascending series” is an influence going from the “purpose” of the whole process (as conceived by *reason*), to its constituent “things” (as objectified by *understanding*). The most immediate illustration of this bi-directional circulation of causes is human goal-oriented action. A tool is an efficient (“descending”) cause of transformations of our environment, whereas our representation of the form of the desired effect is the final (“ascending”) cause of our making and using the tool. By a protraction of reason, a natural system that does *not* result from the intention of a concrete agent can nevertheless be thought of under the *idea* of purpose. This is especially the case of living beings (or “organized beings”), since “(...) an organized being has within it *formative* force, and a formative force that this being imparts to the kinds of matter that lack it (thereby organizing them)” (Kant 1987, 253). Organized beings can be considered as imparting an “ascending” (“downward” according to the current lexicon) influence on their material constituents. Their organization can be taken as imposing a feedback on what is organized. It can therefore be thought of *as if* it were the final cause of the whole process. A. Weber and F. Varela summarized Kant’s lesson by calling *autopoiesis* (which involves the complete circuit of reciprocal causalities,

from parts to whole and from whole to parts) a case of “embodied finality” (Weber and Varela 2002).

These conceptions combining material, formal, and final causes provide us with an elegant ordering scheme of our conception of parts and wholes. But they should not be taken as anything more than that: a satisfaction of our urge for conceptual harmony. Kant himself forcefully pointed this out: Final causality, he wrote, only provides our reflective power of judgment with a *regulative principle* (a compelling guiding thread). By contrast, efficient causality operates as a *constitutive principle* (a condition of possibility of objective knowledge). Then, unlike the category of efficient causality, which is imposed in advance by our *understanding* in order to constitute objective knowledge, final causes are thought of by our *reason* in order to fulfill a subjective need of systematic unity of knowledge (and are also required from our reason by the empirical fact of organismic life).

At any rate, a combination of material, formal and final causality does not solve all the difficulties listed in Section 2. It is still dubious whether stating *separately* the self-imposed boundary conditions and their self-imposing elements, or the global attractor and the self-organizing constituents, is more than a verbal (or heuristic) device. And we still have to give the importance it deserves to the fact that changes at upper levels of organization can *trigger* changes at lower levels.

The persistence of this list of problems is a challenge that can hardly be addressed unless one accepts a minimalist and deflationary conception such as “weak emergence.” Remember that defending weak emergence means claiming that “the system’s global behavior derives just from the operation of micro-level processes, but that the micro-level interactions are interwoven in such a complicated network that the global behavior has no simple explanation” (Bedau 2002, 10). The initial motivation of the conception of weak emergence was to indicate a middle way between strong emergence with its dualist flavor, and purely nominal emergence in which the higher level is nothing more than an artifact of language. But at the end of the day, according to its best supporter, it appears that “weak emergence is (nothing but) a proper subset of nominal emergence” (Bedau 2002, 11; see Bedau 2008a for a qualification). Weak emergence is the special subset of nominal emergence that corresponds to the case where excessive complexity in practice prevents any detailed micro-explanation of macro-behavior. If one retains the latter criterion, it may appear that in most cases “a weakly emergent property is a *limitation of the observer*, not a property of the system” (Batten 2008). A persistent distinction between weak emergence and flat nominal emergence therefore depends



on showing how this limitation of the observer can sometimes be so extreme that it displays the characteristics of an impassable boundary. This may occur whenever the practical limitation in our aptitude to explain macro-behavior is so challenging as to acquire a sort of “in principle” status (Bedau 2008b). This may also occur if many details of the micro-explanations are irrelevant for accounting for the macro-behavior, and if, accordingly, a given macro-explanation can be underpinned by several different micro-stories (Bedau 2002).

No genuine (upward or downward) causation, and ontologically little more than nominal emergence: This is the disappointing outcome of research developed under a substantialist construal of the basic elements. Is there any alternative left? I think there is, provided the substantialist presupposition is dropped at *every single level* of description.

In order to identify this way out I wish to proceed with prudence. Let me first step down, in the next section, from big metaphysical issues about *causality* to practical issues about what counts as a *cause* in a laboratory and in everyday life (Bitbol 2007a).

### 3. An Interventionist Conception of Downward Causation

In ordinary circumstances, we are overwhelmed by the number of antecedents that are likely to have caused a certain event. Among all these antecedents, the one that we usually consider as the cause of this event is either the antecedent that appears to have *changed* recently, or, more convincingly, the one that we can get *control* of (Mill 1851; Pattee 2000). Control, intervention, and action are central touchstones when causes are at stake. This elementary criterion for isolating causes then gives rise to a full-blown conception of causality, called the “interventionist” theory. According to this theory (Von Wright 1974; Price 1992; Woodward 2003; Gillies 2005), configuration A is a cause of the distinct configuration B if: (i) whenever A has been actively set up by any means, B occurs (with probability  $p$ ); (ii) whenever A has been actively removed, B does not occur (or occurs with probability  $p' < p$ ). Interestingly (Ducheyne 2006), this definition of causality was retained by one of the founders of the modern science of nature, Galileo Galilei (1612, 425): “The cause is that which, when posited the effect follows, and when removed the effect is removed.”

We can then speak of “downward causation” in the following circumstances: (i) whenever an upper-level antecedent has been actively set up by means of a “coarse” instrument able to alter macroscopic patterns,

certain elementary phenomena are observed by means of experimental devices designed for microscopic analysis; (ii) whenever this upper level antecedent has been actively removed by “coarse” instruments, those elementary phenomena are not observed. One can define “upward causation” likewise by just inverting the previous order of intervention and observation.

Several difficulties of the concepts of upward and downward causation are formally solved by this theory of causality.

One solution concerns the non-causal (or at least non-*efficiently* causal) status of constraining boundary conditions. Even though the system of mutual constraints or the boundary conditions cannot be considered as causes by themselves, an *alteration* of constraints at one level may cause events at another level. For instance, the constraints set by the mental state of an individual cannot be said to *cause* neural and molecular events in the body of this individual; it is more reasonable, according to the dynamical conception, to consider them as co-extensional. But *actively triggering a change* in this mental state by psychological means may result in changes in her sympathetic-parasympathic balance, thus giving rise to changes in cell metabolism, increased liability to genetic mutations, or activated blood coagulation (Geiser and Halbrecht 2008). If one accepts that causing means *altering* a certain configuration rather than *being* this configuration, one easily makes sense of such psychosomatic phenomena.

This continues to be true when the putative levels are so intermingled that it looks artificial to hold a dualist picture of them. Indeed, each *type of intervention* can be set up in such a way that it (i) concerns specifically and (ii) contributes to *defining* one level of organization, by being more or less coarse-grained and more or less tuned to certain configurations. One can then institute a duality of targets for action, in spite of there being no reason to assume an ontological duality between the levels, and even no reason to think that questions about what levels are “in themselves,” independently of any method of assessment, make sense. The difficulty that arose from the tension between a monist conception of natural processes and the dualist or pluralist vocabulary of “levels” is thus overcome.

The interventionist conception of causality also helps to solve another difficulty, about the temporal succession of causes and effects. Even though the evolution of the higher-level patterns can be taken as simultaneous with the corresponding lower-level processes, the *intervention* itself is prior to any alteration of the targeted pattern. True, an intervention on the macroscopic level does not alter *retroactively* the

micro-conditions from which the macro-level allegedly arose (which would fall prey to Kim's accusation of vicious circularity); but it can alter the micro-conditions for its *future* evolution. The difficulty of the apparent simultaneity of downward causes and their effects thus disappears. Notice that this solution to the time-lag problem formally resembles a proposition of the paradigm of "weak emergence:" "A weak macro-cause cannot alter the conditions from which it arose. At most it can alter the *conditions* for its subsequent survival (...)" (Bedau 2002, 22). However, there is a major difference. In the interventionist conception of causation, the verb "to alter" has the concrete meaning of a disturbance introduced from outside, a disturbance that contributes to defining its own specific target through the scale and "coarseness" of the instrument one uses for triggering it. Instead, in the framework of "weak emergence," the verb "to alter" is used only in order to connect verbally two contingent levels of conceptual or computational analysis of an otherwise unique dynamical process, which concerns a set of interacting "basic elements." No *real* influence is supposed to take place between levels of conceptual or computational analysis. One can *say* that a present traffic jam alters the conditions of the subsequent motion of the cars that compose it. But, admittedly, in the "weak emergence" framework, this is only a way of speaking used in order to compensate for a lack of detailed knowledge, and unable to hide the fact that *ex hypothesi*, *all there is* is a set of cars that at each instant move according to the distance of their immediate neighbors.

#### **4. Interventionist View of Downward Causation: First Objections and Replies**

As long as one sticks to a substantialist construal of the basic elements, however, the tentative solution offered in the previous section is bound to look parochial or anthropocentric. Indeed, in this framework of thought, action, intervention, and higher levels of organization as well, are all supposed to be derivative when compared to the basic constituents. Accordingly, Von Wright's theory of causality is usually taken as only epistemological, not ontological; it is supposed to clarify the way we happen to *know* causes, not what causes *are*.

As for the idea that intervening at a high level of organization may be the genuine *cause* of changes at a lower level, it raises at least two objections. Firstly, it may be replied that saying that one has imposed alterations to a given high level of organization is only a way of expressing one's ignorance of the detailed microscopic changes that have been triggered *in reality*. Secondly, it may be argued that the so-called

high-level cause of a subsequent change at a lower level is at most a *releasing* cause of this alteration, not its *integral* physical cause, which is likely to involve the entire network of interactions between the basic constituents.

These objections are easily met within another framework of thought, which I would like to characterize as *conceptually symmetric*.

The standard conception of emergence is characterized by a twofold asymmetry:

- (i) The usual picture of emergence is asymmetric because it assumes that the basic level is made of individual entities, whereas the higher levels are made of structures, or patterns.
- (ii) The usual picture of emergence is also asymmetric because it assumes that the determinations of the basic level are “properties,” in so far as they are “proper” to, or inherent to, the elementary entities, whereas the determinations of the higher levels are *relative* to certain (contingent or necessary) *limitations* of the cognitive instruments used to assess them.

But, in view of recent developments of modern physics, both asymmetries appear unwarranted in principle.

On the one hand, in quantum physics, it can hardly be assumed that there is an ultimate basic level of processes made of individual little things able to interact with one another (Bitbol 1996, 2007b). Setting aside any conceptual trick such as hidden variables, the so-called elementary particles have to be treated as non-individuals, as mere units of a limited set of “sorts,” and thus as formal rather than substantial entities. This becomes even clearer in Quantum Field Theory, where cardinals of subsets of particles are in one-to-one correspondence with quantized modes of excitation of fields (Teller 1995). Accordingly, particles are *de facto* treated as patterns or configurations, rather than as substantial entities (Bickhard and Campbell 2000). The analysis of a level of organization in terms of structures, patterns, and topological configurations imposes itself throughout the scale of levels, *even at the lower accessible level* (Campbell and Bickard 2009). The first asymmetry of the standard picture disappears thus.

On the other hand, in quantum physics, one can no longer overlook the fact that determinations are exclusively relational or contextual. Here, the cognitive relation cannot be taken as merely revealing, but as *constitutive*. This circumstance pushes the so-called “basis” of emergence surprisingly close to the higher levels of organization. The determinations of the

lower-level entities are just as much *relative* to certain *limitations* of the appropriate cognitive instruments as those of the higher-level entities. The only difference is that the limitations of the cognitive instruments are impassable in micro-physics, whereas they can in principle be overcome (notwithstanding complexity) at higher levels of organization. This latter difference may explain why it is tempting to privilege microscopic physics, but it does not justify forgetting the universality of the mode of definition of attributes relative to a mode of experimental access. Once this universality is recognized, the second asymmetry of the usual picture disappears too.

Without any ontological asymmetry, without any stubbornly substantialist construal of the so-called “basic” level, the dignity of the interventionist conception of causality is dramatically improved. On our construal, it becomes pointless to maintain a distinction between epistemological and ontological conceptions of causation, since nowhere can one point towards something like an ultimate inherent property that sets the standard of ontology. At every level, the cognitive relations and the experimental interventions are constitutive of their object and of their target respectively. Therefore, it is not correct to claim that what is described as an intervention on a higher level of organization is *in reality* an intervention on its elementary parts. For these putative parts are no more inherently real than the upper levels of organization; they are just as much relative to a certain mode of investigation or action as these upper levels. At most, one can say that intervening on a high level of organization means acting on a domain of cognition that *would* be analyzed into parts *if* a microscopic mode of intervention were used instead. But this counterfactual statement should not be mixed up with an ontological statement about the elementary parts. For the analytic activity relative to which the parts are defined is likely to be *exclusive* of another activity performed at an organismic or global level (see the next section for an example of mutual exclusivity).

Similarly, it becomes pointless to make a distinction between the releasing cause of a certain alteration and the “physical” cause. For, in our symmetric framework of thought, the releasing cause is not only triggered but also *constituted* by an appropriate intervention. And the physical (microscopic) cause is evoked only by counterfactual reference to a network of factors that *could* have been constituted by another (possibly incompatible) type of intervention.

## 5. A Quantum Model of Downward Causation

An illustration of this symmetric and interventionist conception of downward causation will now be given by examining a familiar quantum mechanical model. The motivation for displaying this kind of model is that in standard quantum mechanics, the ideas that observables are operationally defined and that experimental interventions are *co-constitutive*, rather than merely revealing of properties, are built into the theory.

Let us concentrate on the state vector of a two-particle system in which each particle (each sub-system) can be submitted to an elementary two-values experiment (such as measurement of a component  $s_z$  of spin  $1/2$ ). The possible outcomes of the measurement are labeled  $+$  and  $-$ , and the corresponding eigenstates of observable  $s_z$  are:  $|+\rangle$  and  $|-\rangle$ .

The generic state vector of a two-particle system then takes the form of a linear superposition of tensor products of these eigenstates:

$$|\Psi^T\rangle = \sum_{ij} c_{ij} |ij\rangle = c_{++} |++\rangle + c_{+-} |+-\rangle + c_{-+} |-+\rangle + c_{--} |--\rangle$$

This state vector  $|\Psi^T\rangle$  is usually not factorizable. The contributions of the two subsystems cannot be set apart; they are said to be “entangled.” According to Schrödinger (1935/1983), who first formulated the concept of entanglement, this means that “[b]est possible knowledge of a whole does not necessarily include (best possible knowledge of) its parts. (...) The whole is in a definite state, the parts taken individually are not” (161)

A precise way of displaying this type of relation of parts and wholes in quantum mechanics consists in comparing different states of the two-particle system taken as a whole, and demonstrating that these differences have no counterpart whatsoever in the individual states of the sub-systems.

To show this, let us first consider four mutually orthonormal (entangled) states.

$$\begin{aligned} |\Psi^+\rangle &= 2^{-1/2} (|+-\rangle + |-+\rangle) \\ |\Psi^-\rangle &= 2^{-1/2} (|+-\rangle - |-+\rangle) \\ |\Phi^+\rangle &= 2^{-1/2} (|++\rangle + |--\rangle) \\ |\Phi^-\rangle &= 2^{-1/2} (|++\rangle - |--\rangle) \end{aligned} \quad (1)$$

These are global states for the two-particle system. But what about the individual states of the sub-systems? These individual states cannot be denoted here by a state vector. At most, one may associate each sub-system with a *density operator*  $\rho$ , obtained by taking the *partial trace* of the matrix representing the density operator of the two-particle system. The problem is that these individual density operators are *exactly identical* to each other, irrespective of the whole system's being in any one of the former four states. They *always* write:

$$\rho = 1/2 (|+\rangle\langle+| + |-\rangle\langle-|) \quad (2)$$

Therefore, there exists no difference in the states of the parts that may account for the difference in the state of the whole (Maudlin, 1998). *The differences in the state of the whole are not supervenient on corresponding differences of the parts.* This is one of the most remarkable holistic-like features of quantum mechanics among those used by P. Humphreys (1997) to develop his conception of strong emergence based on what he called “fusion” of micro-properties (Seevinck 2003).

Another, less documented consequence of entanglement is that any attempt at *separating completely* the states of the parts from the state of the whole is bound to fail. This sounds strange, since we have accepted (at least tentatively) that the state of each component particle (or sub-system) of a two-particle system can be described separately as a density operator. But the latter kind of density operator is quite peculiar: Using the terminology of B. d'Espagnat (1989), it corresponds to an *improper* statistical mixture, not a *proper* mixture. Not all the relevant information about the sub-system is contained in its density operator (obtained by *partial tracing*). A fraction of this information is missing, and it is contained only in the state vector of the overall system. Any separate description of parts, and then any *dual* description of parts and whole, then looks artificial.

As a consequence, the concept of inter-level causation looks nonsensical in the highly holistic domain described by quantum mechanics. Since there is no way to separate the states of the parts from the state of the whole, it sounds absurd to call one the cause and the other the effect, as if they were two different things.

Now, even though one cannot separate the contribution of the parts and of the whole within an entangled state, there is a sense in which one can *intervene* selectively either on the parts or on the whole. For one can *intervene* either analytically or globally. Measuring individual observables (or preparing sub-systems in eigenstates of such observables) is

tantamount to intervening on the parts; whereas measuring global observables (or preparing a system in an eigenstate of such an observable) is tantamount to intervening on the whole. Thus, measuring the component  $s_z$  of the spin of each particle belonging to a two-particle system means intervening on its parts. But preparing this two-particle system in one eigenstate of a global observable (in a 4-dimensional Hilbert space) means intervening on its whole. In order to display the consequences of this distinction, let me give a new list of eigenstates corresponding to an interesting global observable. This list is made of one “singlet” and three “triplet” states (Cohen-Tannoudji et al. 2006):

$$\begin{aligned}
 (\text{Singlet}) \quad & |\Psi^-\rangle = 2^{-1/2} (|+-\rangle - |-+\rangle) \\
 & |\Phi^0\rangle = |++\rangle \\
 (\text{Triplet}) \quad & \{ |\Psi^+\rangle = 2^{-1/2} (|+-\rangle + |-+\rangle) \\
 & |\Phi^1\rangle = |--\rangle \}
 \end{aligned} \tag{3}$$

If a two-particle system initially in state  $|\Psi^T\rangle$  is prepared in state  $|\Psi^-\rangle$  or  $|\Psi^+\rangle$ , we can be sure that local measurements of the individual observable  $s_z$  performed on the two sub-systems will yield one + and one -. And if a two-particle system initially in state  $|\Psi^T\rangle$  is prepared in state  $|\Phi^0\rangle$  (respectively  $|\Phi^1\rangle$ ) we can be sure that local measurements of the individual observable  $s_z$  performed on the two sub-systems will yield two + (respectively two -).

This means that *intervening on the whole has effects on values of observables bearing on the parts*.

In other terms, preparing a two-particle system in a certain state of a global observable amounts to a variety of *downward causation*, since this determines the distribution of values one may subsequently obtain if local observables (such as  $s_z$ ) are measured separately on the sub-systems. Global preparation *downwardly causes* a distribution of values of local observables. The converse also holds, of course. If we measure the values of the local observables  $s_z$  on the sub-systems first, and get the outcomes  $i$  and  $j$ , then by measuring the global observable “total spin” one can find the system only in the factorizable state  $|ij\rangle$ . Local measurements here *upwardly cause* a global state.

Notice that an intervention on the whole can by no means be identified with a coarse-grained action that “in reality” bears on the parts. Indeed:



- (i) In standard quantum mechanics, relations with experimental devices are *constitutive* in the strongest sense: They determine generically which observable is concerned (global or local), and individually which value of this observable is realized.
- (ii) Global observables and local observables generally do *not* commute with each other. The global observable associated to the list of eigenstates (3) thus does not commute with the local observables  $s_z$ . Therefore, the constitutive act corresponding to measurement of a global observable is generally *incompatible* with the constitutive act(s) corresponding to measurement(s) of local observables.
- (iii) As a consequence of points (i) and (ii), the values of local observables generally cannot even be ascribed any *counterfactual definiteness* when the value of a certain global observable is defined and obtained by appropriate measurements.

According to (iii), the conditions that allow ascription of a global property to a quantum system generally *exclude* the conditions that allow ascription of local properties. If a global property is defined and ascribed, *it is then wrong to say that there exist underlying local properties on which one is acting "in reality."*

The non-dualist and anti-foundationalist features of this quantum model are obvious at this point. Let us recapitulate them:

- (a) The holistic-like character of the state representation of quantum systems makes any two-level description of these systems look artificial.
- (b) In this representation, one cannot even use the usual concept of supervenience to reconcile the ideas of dependence (of the global level on the local level) and autonomy (of the global level with respect to the local level). Indeed, there may exist differences between global states without any corresponding differences between the local states that are supposed to underpin them.
- (c) Properties and states cannot be treated as preexistent intrinsic features. They must be construed as relational. Properties are thus replaced by "values of observables," in so far as they are relative to particular instantiations of measurement acts.
- (d) Experimental interventions simultaneously single out and *define* a type of property: global properties are defined relative to the measurement of large-scale observables, and local properties are defined relative to the measurement of low-scale observables. The conditions relative to which global observables are defined generally

*exclude* the conditions relative to which local observables are defined.

- (e) Upward and downward causation make good sense as soon as one does not pay too much attention to state representations, and focuses on the effect of (local or global) experimental *interventions*. Measuring or preparing global observables may influence the results of later measurements of local observables, and conversely measuring or preparing local observables may influence the results of later measurements of global observables.

Points (a) and (b) dispel dualism of levels, and points (c) and (d) challenge foundationalism. As for point (e), it elaborates on the status of downward and upward causation in a non-dualist and anti-foundationalist framework.

## 6. About Some Possible Misunderstandings

The conception of downward causation developed in the previous sections, which we may now call the “interventionist-constitutive view,” is unfamiliar enough to trigger misunderstandings. The purpose of this section is to dispel some of them.

The first misinterpretation concerns the role of quantum-mechanical concepts in my defense of the interventionist-constitutive view of downward causation. The central argument adduced to defend the interventionist theory of causality against the accusation of anthropocentrism in Section 5 was borrowed from the philosophy of quantum mechanics, and even quantum field theory; but is it really indispensable to rely on such far-fetched and allegedly exotic domains of physics? The quantum model presented in Section 6 has features that make inter-level causation plausible; but is it representative of more standard cases of downward and upward causation? Here are some tentative answers.

In the argument of Section 5, relying on the philosophy of quantum mechanics seems to be a contrived strategy only because one forgets that one is dealing with matters of *principle*. The problem here is whether or not there is *in principle* a difference between “ontological” causes and a “purely epistemological or anthropological” definition of causality. Claiming that there is indeed such a difference presupposes a distinction between: (i) lower levels of *basic individual constituents* where the experimental intervention procedure helps us to *reveal* the true causes identified with micro-properties of individual constituents, and (ii) upper levels of *organization* where the experimental intervention can trigger a

chain reaction of real micro-causes only by coarse alteration of their global pattern. So, what about the validity of this distinction postulated by the view I am criticizing?

Consideration of intermediate levels is of little help for addressing such a question. Indeed, any intermediate entity (such as a molecule, a cell, an organism, etc.) can be seen indifferently either as an elementary individual constituent of the upper level of organization, or as a pattern emerging from the lower level of organization. Accordingly, an intermediate entity can be construed either as an unquestioned (and therefore *de facto* absolute) elementary building block for the upper levels of organization, or as relative to the coarse mode of access that singles out its own level of organization. An intermediate entity can also be taken either as the real elementary cause of a certain process taking place at some upper level of organization, or as a coarse target for interventions meant to trigger events at its own level of organization (or at lower levels). In other terms, consideration of intermediate levels can display only *functional* or *instrumental* asymmetry between basic elements and emergent patterns. Intermediate levels present us with no motive to declare that there is a *fundamental* and *irreducible* difference between: (i) absolute, ontological, efficient causes, and (ii) relative, epistemological, releasing causes at higher levels defined (nay *constituted*) by a scale of experimental intervention. Actually, every such intermediate level falls under the second (relative, epistemological, releasing) category of causes, and it is only by reference to upper levels that one can conventionally (and provisionally) grant it the *role* of a repository of basic entities and real causes.

The only unshakable reason for taking seriously the distinction between the two types of causes, and for accepting that there is a difference of *principle* between an ontological and a purely epistemological-anthropological conception of causes, would then be to have the assurance that there exists an *ultimate* basic level of individual entities endowed with intrinsic properties. For, then, these micro-properties would inherently count as real causes, and any other higher-level process circumscribed as a target for macroscopic action could give rise *only* to “epistemological” or “relative” releasing causes. Unfortunately (for this way of thinking) micro-physics has strong arguments in store against such a concept of an ultimate basic level, because, (a) as I mentioned in Section 5, the so-called “elementary” particles are replaced by quantum field patterns, and also because (b) *not even* quantum fields can be considered as basic entities, since they all appear (in view of *renormalization*) to be nothing more than “effective fields” for ever deeper levels of field-

theoretic entities (Hartmann 2001; Castellani 2002). Therefore, at *no* level, even the deepest and (presumably) most elementary level of micro-physics, are there anything like absolute properties and absolute causes to be opposed to the (so-called) anthropological, epistemological, relative causes that can be defined by varying the scale of intervention on putative antecedents. There is *no* cause that one could consider as a “primary quality” of matter; every cause arises as a “secondary quality” in so far as it is relative to a certain procedure of intervention (Menzies and Price 1993). In the absence of any contrast of this kind *even in the putatively ultimate domain of micro-physics*, the interventionist definition of causes is bound to become paradigmatic *in principle*, not only *in practice*.

A second possible misunderstanding is to think that the example developed in Section 6 is an exceptional case of downward causation, which works only in the unique epistemological configuration of quantum mechanics. This example is in fact less isolated and less exceptional than it may appear. Indeed: (i) the epistemological features of quantum mechanics represent only a reinforced version of a universal situation, and (ii) there are some non-quantum cases that fully implement these epistemological features in their reinforced version.

About point (i), even classical physics can be seen as instantiating a type of science that only deals with some sort of “secondary qualities” and *never* with “primary qualities.” This was Kant’s interpretation. In his *Prolegomena*, he insisted that even spatial and kinematic predicates can (and should) be considered “secondary” in Locke’s sense (Kant 1955, §13). They should be considered secondary because they are relative to the pure form of our *sensibility*. By extension, Kant could have said that ascribing something the status of a “substance,” or the status of a “cause,” is also to be considered as “secondary,” because both ascriptions are relative to the pure form of our *understanding*. The strategy of universalization of relational/contextual predicates in every domain and at every level can thus already be defended in classical science, against the substantialist and foundationalist conceptions which underpin reductionist approaches of interlevel relations. This strategy is still used nowadays, in the framework of the autopoietic (Maturana and Varela 1980) and “ecological” (Gibson 1979) theories of cognition, in biosemiotics inspired by Von Uexküll’s theory of *Umwelt* (Hoffmeyer 1997), etc.

About (ii), it is now increasingly recognized (Lambert et al. 2006; La Mura 2005; Atmanspacher et al. 2004) that certain domains of human sciences (economy, psychology of perception, rational choice theory, etc.) share *exactly the same* (and not just analogous) characteristics and backbone structure as quantum mechanics. The reason for this strong

similarity is simple to understand: In all these cases, just as in micro-physics and unlike macro-physics, the predicates cannot be disentangled from the methods of access or from the agents (Bitbol 2009b). The most basic mathematical structures of quantum theory can then be transposed to these domains, including those involved in non-factorizability of state vectors. Generalized quantum formalisms able to apply beyond the realm of physics have been formulated, and applied with success to several situations in the human sciences (Atmanspacher et al. 2002).

For all these reasons, the quantum case of interventionist-constitutive downward causation discussed in Section 6 is likely to have a much higher degree of generality and relevance than expected.

A third misunderstanding may arise about the topic of *intra*-level causal powers. These have just been ignored in this article until now, in favor of a systematic study of inter-level causation. Has the interventionist-constitutive conception of causation anything to say about intra-level influences? Besides, if (as the interventionist-constitutive conception requires) one grants an equal status to high-level *intra-level* causes and to low-level *intra-level* causes, isn't there a redundancy of causes? How can one reconcile this equality of status between high-level and low-level causes with the idea of *causal closure* of the domain of physics?

The first question can be answered unambiguously in the positive. The interventionist-constitutive conception of causation is indeed applicable to the case of intra-level causation. For this, it is enough to consider that both the instrument of intervention and the instrument of observation are designed for targeting (and thereby co-defining) the same level. The two clauses that define an intra-level cause according to the interventionist conception are then the following: (i) Whenever an antecedent has been actively set up by means of a level L-specific instrument  $I_{L+}$ , certain phenomena of level L are observed; (ii) whenever this antecedent has been actively removed by another level L-specific instrument  $I_{L-}$ , the former phenomena of level L are not observed.

Now, in order to answer the second question, one has to take seriously the word "constitutive" in the expression "interventionist-constitutive conception of causation"; just as seriously, in fact, as in Kant's theory of knowledge. There, the principles of understanding are constitutive of objects in so far as they are conditions of possibility (or necessary presuppositions) for organizing "rhapsodies of sensations" into objective knowledge. In our case, using the word "constitutive" is meant to express: (i) the relativity of any causal scheme to the method of active substitution of antecedent by means of various instruments adapted to various scales

or levels, (ii) the thesis that, therefore, any causal scheme has these methods and instruments as a necessary presupposition, and (iii) the conviction that *there is no “fact of the matter” as to which of the many instrument-relative causal schemes is more “real” than another*. No level of organization can claim any privilege for itself, because every such level is defined (or “constituted”) by a certain scale of intervention and observation. Moreover, no absolute meta-observer, no “view from nowhere,” is available to select one pattern of causes at a certain agent-relative level as the “truly efficient” one. This does not threaten the thesis of causal closure of the domain of physics, but only denies it any ontological significance. Causal closure here means only that it is possible to establish a systematic and self-sufficient network of causal connections relative to a single scale of intervention and experimental access, without having recourse to any other scale of intervention and access. This being granted, causal closure of a low level of organization (say the level of micro-physics) is perfectly compatible with the thesis that there are also efficient causes at an upper level of organization. Causal closure at one level shows only the efficacy and reasonable exhaustiveness of the procedures of intervention and access that define this level, in yielding a coherent picture *relative to these procedures*. Nothing then prevents one from obtaining another coherent picture, possibly with causal closure, at another level and with other procedures of intervention and access. These two internally coherent pictures and causal closures can *both* be valid, each at its own level, and relative to its own set of procedures of intervention and access. Far from being mutually exclusive (as an ontological conception of causation would require), they can be made mutually consistent. Of course, mutual consistency here does not mean that they are somehow identical, but only that they are *inter-translatable*, as if they were two different languages (say a micro- and macro-language).

For instance, according to the old-fashioned dogma of molecular biology, one can say that:

- (a) A gene *causes* a phenotypic feature of the cell.
- (b) A DNA strand’s opening offers regions of selective affinities for nucleotide basis, RNA polymerase moving along the DNA then *causes* successive pairing of the nucleotide basis of mRNA with the nucleotide basis of DNA (this is called “transcription”), and finally mRNA, along with ribosomes and transfer RNA, *causes* systematic pairing with amino-acids thus resulting in a certain protein primary structure (this is called “translation”).

In this standard framework, the biological-genetic causal scheme (a) does not exclude the chemical-molecular causal scheme (b), nor conversely; it is compatible with it under certain rules of (complete or incomplete) inter-translation. These inter-translatable causally closed schemes are not even redundant. Indeed, each one of them is indispensable relative to the corresponding procedure of intervention and access. In the framework posited by *this procedure*, it could not be replaced by another causally closed scheme without loss in explanatory power.

## 7. Downward Causation beyond Present Interventions

Another challenge to the interventionist conception must be addressed at this point. Is there a sense in which an event at a certain level L can be said to cause an event at the lower level l, *even in the absence of a present intervention* at level L? As we will now see, this question can be answered without reference to “causes in themselves,” by studying the mode of interconnectedness between *domains of knowledge defined relative to different modes of access and concepts*.

L. Bich (2009) recently formulated this strategy, with inspiration from R. Rosen’s (1991) concepts of scientific models and relational biology. To begin with, one notices that it looks nonsensical to posit real interactions between entities of two models (say a high-level and a low-level model) of a certain process, since each model is relative to a completely distinct class of modes of access and modes of conceptualization. Figuring out interactions between such entities resembles Ryle’s “category mistake.” However, there are special kinds of operations that may set the conditions for an indirect comparison between the domains ruled by the two types of models. These operations aim at defining entities of the *same category*, yet starting either from the high level or from the low level. These operations are, respectively, *analysis* and *synthesis*. Analysis is a top-down procedure starting from the higher-level system S and trying to figure out its parts (or its “components”). Synthesis is a bottom-up procedure that starts from “material elements” (whose concept is derived from a model of the basic physical level), and tries to elaborate a model of something like system S as the final outcome. In simple linear systems, the “components” obtained as a byproduct of analysis, and the material “elements” taken as starting points of synthesis, coincide. But in many other cases, this is not true. The model of the whole so to speak imposes a mark on its components, making them different from the alleged basic material elements. Downward causation is then defined as the *non-*

coincidence of the models that apply to the components of a system with the models of its material elements; or as *the non-coincidence of the end product of the operation of analysis with the starting point of the operation of synthesis*.

Let me give an example, borrowed from quantum chemistry (Hladik 1971; Vemulapalli 2003; Bensaude-Vincent 2005). If one starts from a quantum model of an isolated atom of carbon, one can predict neither its valence nor the geometry of its possible chemical bonds. The model of electron distribution of the atom of carbon taken in isolation is indeed:  $[1s^2, 2s^2, 2p_x^1, 2p_y^1, 2p_z^0]$  (two electrons on the layer 1s, two electrons on the layer 2s, one electron on each of the layers  $2p_x$  and  $2p_y$ , and no electron on the layer  $2p_z$ ). This electron distribution entails the *di*-valence of carbon (because only two electrons are unpaired: those on layers  $2p_x$  and  $2p_y$ ), and an angle between the two predicted bonds equal to  $90^\circ$ . But this is almost always wrong. Methane and other molecules including carbon display the *tetra*-valence of carbon atoms, and a tetrahedral geometry with an angle between the bonds close to  $109^\circ$ . In view of this huge discrepancy, quantum chemists then introduced the *ad hoc* trick of “orbital hybridization.” The states of the two electrons on layer 2s were linearly combined with the states of the electrons on  $2p_x$  and  $2p_y$ , and one then obtained four unpaired electrons in hybridized states called  $sp^3$ . This finally accounted for the observed molecular structures. It is clear at this point that the physical model of the isolated carbon atom taken as the starting point of bottom-up synthesis does not coincide with the chemical model of carbon-components of molecules that is the end product of top-down analysis. The bottom-up *elements* ( $2s^2 2p_x^1 2p_y^1$  - isolated carbons) do not coincide with the top-down *components* ( $sp^3$  - hybridized carbons). This non-coincidence between bottom-up and top-down procedures and associated models accounts for what we may call a case of “downward causation,” *beyond the situation of an immediate intervention*.

Here again, it is tempting to forget the whole cognitive procedure and jump to the claim that ontologically construed molecules have an influence on ontologically construed atoms. One could say, for instance, that molecules of methane downwardly influence carbon atoms by altering their electron distribution, changing it from the  $2s^2 2p_x^1 2p_y^1$  configuration to the  $sp^3$  configuration. But this shortcut immediately raises all the objections listed in Section 2. By contrast, mere non-coincidence of bottom-up and top-down experimental *procedures*, and of the two corresponding *models* of the lower level, is immune to these objections formulated in an ontological framework.



To sum up, according to the interventionist-constitutive view, there is a sense in which an event at a certain level *L* can be said to cause an event at the lower level *l*, even in the absence of a *present* intervention at level *L*. This requires only understanding how patterns of experimental interventions are used to formulate permanent law-like statements, and connecting various access-relative models.

## 8. Downward Self-causation

A crucial question is still left over at this point. We have seen that downward causation makes perfectly good sense when an *external* intervention at a given organization level which is at the same time targeted and defined by it, induces alterations observed at a lower level. Now what about *self*-intervening and *self*-altering? This notion sounds nonsensical. Self-alteration looks like a verbal trick for expressing mere unobstructed evolution of a process. However, everybody knows cases of (apparent or real) self-interventions in which a voluntary change of state of mind has an influence on one's own physiology (Petitmengin et al. 2006).

The major sticking point concerns the word "voluntary" in the expression "voluntary change of one's own state of mind". Are we *really* free to change our state of mind? More generally, are we *really* free to choose any one of our actions (Libet et al. 1999)? Even before examining this question, its underlying presupposition must be exposed. The very fact that the debate bears on the *reality* or *irreality* of free will is a further symptom of the dominance of a foundationalist framework. Those who argue in favor of the reality of free will tend to ground it on a reified conception of mind. And those who argue *against* the reality of free will tend to reify objective descriptions of physiology and behavior (Bitbol 2008a, b). The latter authors are prone to accept that our experience (especially our experience of free will) may be an illusion, whereas the law-like objective description of the functioning of our body exposes its *real* working. However, if Kant's "Copernican revolution" is pushed to its ultimate consequences, this kind of cut between experiential illusion and *intrinsic reality* as disclosed by inquiry appears to be an even deeper illusion, generated by reason's mistaking its own horizons of research for metaphysically real entities (Kant 1996).

An alternative pluralist and access-sensitive analysis of free will is then needed. It develops in two steps. Firstly, one dispels carefully the classical dualist view which is inadvertently associated with the phrase

“free will”; to wit the idea that free will means unruly action of a substantial mind *on* another substantial something. Secondly, one formulates a non-dualist alternative to this misleading metaphysical picture. An interesting account of this kind, adapted from Kant’s *Critique of Practical Reason* with a touch of Spinozism, relies on the dialectic of the actor and the spectator (Beck 1963). The spontaneous belief in free will here arises from the standpoint of an *actor* immersed in nature, whereas denying free will is unavoidable from the standpoint of a *spectator* who undertakes to posit part of this nature as an object of description. According to Kant (2002), even though there can be no “theoretical” proof of freedom (i.e., no proof from the standpoint of a spectator), things are different from the standpoint of the actor. Indeed, someone “(...) cannot *act* except *under the idea* of freedom” (247); and this entails that *in some sense* one is “*really* free.” One must insist at this point on the unusual but sensible reasoning of Kant:

- (i) In order for the very process of *deliberation* to develop and make sense, actors must work under the unquestioned *presupposition* of free will. As a counterexample, let us imagine an actor who decides to do something, but suddenly realizes that, at any rate, what she will do next is already pre-determined. This implies a lived *performative contradiction* (Apel 1984) that, if (too) consistently taken into account, may result in inhibition of the decision and mere passivity.
- (ii) This necessary *presupposition* of free will is enough to declare that actors are “really” free from a *practical* standpoint.

The fact that, from the standpoint of a scientific external *spectator* (or even from the standpoint of the same human being who has adopted retrospectively a spectator-like stance towards her own past actions and experiences), the behavior of the agent may appear to be governed by objective deterministic laws does not weaken in the least the practical *reality* of the presupposed freedom. For, here, using the adverb “really” does not require reference to anything else than the spontaneously felt, and in practice indispensable, *presupposition* of deliberative action. This sense of the word “reality” can be considered “weak” only if one forgets that, in a deliberately non-metaphysical view, no “stronger” *a sich* sense is available. In particular, the theoretical sense of the word “reality” can hardly be considered stronger, since it refers only to phenomenal invariants used as practical guides for an intersubjectively coordinated research.

This can be called a “two-stance,” as opposed to a “two-substance,” account of free will: actor stance/spectator stance, instead of spiritual substance/material substance. On the basis of this account, one could say (in agreement with my initial formulation of the status of downward causation) that free will is neither illusory nor inherently existent, but merely indexical or situational. It holds in the situation of an actor, *qua* indexed by this situation.

In particular, there is indeed a sense in which one: (i) can voluntarily alter one’s own state of mind, and (ii) observe the objective physiological “effects” of this voluntary “downward” alteration. No “disruption of the laws of nature by a spiritual substance” is needed for that. It has only to be accepted that step (i) expresses what is presupposed by oneself as an actor (and is then “real in practice”), whereas step (ii) expresses the outcome of an objective science developed by adopting the stance of spectators (and is then “real in theory”).

Finally, one can think of yet another case, which is rarely discussed: “indirect self-influence,” beyond “direct self-causation.” As pointed out by J. Elster, when we wish to alter our own (psycho-physiological) state, it is often better to act indirectly by choosing to influence ourselves laterally, rather than to act directly by trying to cause the sought state. For instance, when we wish to sleep, it is better not to strive towards this aim, but rather influence ourselves by promoting other (apparently unrelated) processes, such as concentration on a repetitive mental task or renunciation of any aim whatsoever. The altered state thus arises as something that is “essentially” an indirect by-product of the promoted process, rather than being a direct effect of our desire to reach it.

It goes without saying that, just as causing, influencing by self-intervening at a certain level contributes to *defining* this level of organization. Accordingly, downward influence holds exactly in the same sense as downward causation by external intervention or by voluntary self-alteration: it holds *qua* indexed by a mode of access and a mode of (lateral) action.

## 9. Conclusion and Summary

- (1) Making sense of upward and downward causation does not require acceptance of some sort of metaphysical distinction between the higher and basic levels of organization: neither a substantial distinction as in genuine dualism, nor a distinction between properties and structures as in the current popular picture. It is

enough to assume a duality of modes of access, or modes of intervention.

- (2) If one intervenes at a higher level of organization, some effects of this action can then be detected by a mode of access specifically aimed at a lower level. This is downward causation. Conversely, if one intervenes at a microscopic level, some effects of this action can then be detected by a mode of access specifically aimed at a higher level of organization. This is upward causation.
- (3) The modes of access and the modes of intervention are not just revealing; they are *constitutive* throughout. Accordingly, the levels of organization are not only disclosed but also *defined* by corresponding modes of intervention.
- (4) Therefore, saying that some intervention at a higher level *downwardly causes* alterations detected at a lower level (or, conversely that some intervention at a lower level *upwardly causes* alterations detected at a higher level) is an accurate expression of a dual mode of *operational definition* of the levels.
- (5) The dual mode of operational definition of the levels can be extended beyond the very moment of intervention, and beyond the simple case of external interventions, thus also making sense of cases of permanent inter-level influence or self-transformation.
- (6) The emergent levels of organization, and the inter-level causations as well, are neither illusory nor ontologically real. They are *objective* in a transcendental, constitutive, sense.
- (7) Alternatively, one can say that the usual dichotomy between epistemology and ontology collapses, because we can ascribe no other meaning to the “being” of levels of organization and causes than that which has been constituted and objectified by an epistemic method of access.

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# THE SIGNIFICANCE OF STRUCTURE: QUANTUM CHEMISTRY AND ORGANIC SYNTHESIS

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## Introduction

Given their disparate aims and divergent histories, it should not be too surprising that the contemporary literature in chemistry and philosophy shows little overlap. Most of those episodes from the history of chemistry that excite general philosophical interest (such as the Chemical Revolution and Atomism) are rather far removed from the concerns of contemporary chemists. Likewise, the research reports of modern chemists are often inaccessible to all but closely related specialists, much less to professional philosophers. Still, some chemists do have their philosophical moments, particularly when reflecting on the significance of their field and its relationship to the broader scientific enterprise. Similarly, several philosophers have made use of developments in relatively contemporary chemistry in order to provide concrete context to more abstract philosophical issues.

As far as I can tell, the locus of what little overlap there has been between these fields is a short quote from P. A. M. Dirac:

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. (Dirac, 1929)

Dirac's claim was made in the context of a description of the then newly developed techniques for treating the quantum mechanics of many-electron systems, such as molecules. His claim has been understood by philosophers to report the successful in-principle *reduction* of chemistry to

physics<sup>1</sup>. *Reduction* is a philosophically loaded concept; both what it means and whether Dirac's report is plausible have been the subject of much of the relatively scant (but growing) literature in the philosophy of chemistry. Mainstream philosophers, on the other hand, have been much more willing to take Dirac's claim at face value, concluding, for instance, that quantum mechanics has succeeded in "unifying chemistry and physics to the extent that the disciplinary boundaries between them now largely reflect historical contingencies and convenience rather than deep conceptual differences" (Sarkar, 2008, p. 431).

In the chemical literature, Dirac's quote is regularly invoked in reflections on the prospects for quantum chemistry<sup>2</sup>. In contrast with philosophers, quantum chemists do not read Dirac's claim as a starry-eyed, in-principle claim about the unity of the sciences, but instead seem to be particularly stuck by Dirac's pessimistic assessment of the prospects for solving the equations. The advent of the digital computer and the development of an arsenal of approximate methods has "overcome to a significant degree the difficulties referred to by Dirac" (Levine, 2009, p. 718), or alternatively, has "made this pessimistic statement obsolete" (Veszprémi et. al., 1999, p. ix). It seems, then, that these quantum chemists not only don't doubt that the mathematical theory of the "whole of chemistry [is] completely known," but also think that they can implement this theory in practice, at least in certain cases.

Needless to say, many other chemists are not as sanguine about the prospects for quantum chemistry. Though it is virtually impossible to find a chemist who fails to recognize and appreciate the strides made in quantum chemistry since Dirac's time, there are some more resistant to the idea that the whole of chemistry has been, or could be, subject to mathematical laws though quantum mechanics. Resistance seems strongest, not surprisingly, in those subfields of chemistry with an experimental, constructive focus, such as synthetic organic chemistry. While acknowledging the important contributions that quantum chemistry has made to synthetic organic chemistry, for example, organic chemists have claimed, "quantum mechanical calculations have not yet become daily working instruments in chemical practice and it is hardly to be expected that this approach might ever become a universal tool for the solution of chemical problems" (Smit et. al., 1998, p. 456). One gets the

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<sup>1</sup> See (van Brakel, 2000, p. 119-150) for both a summary of the philosophical uses of this quote, as well as a catalog of the various contexts in which chemists appeal to it.

<sup>2</sup> See, for instance, (Levine, 2009, p. 718) (Hegre et. al., 1986, p. 1) (Veszprémi et. al., 1999, p. ix).

sense that chemists of this stripe resent the idea that the appropriate measure of the rigor, or theoretical development, of their science is the extent to which quantum mechanics can be brought to bear on the problems in the field. Organic chemistry, they argue, is a rigorous, theoretically well-developed discipline whose distinctive problems and approach aren't going to suddenly disappear when the computers get faster<sup>3</sup>.

For their part, quantum chemists do not typically characterize their aspirations as imperial — aiming for the eventual replacement, or obsolescence, of other parts of chemistry. Rather they too seem more concerned with the epistemological status of their own discipline<sup>4</sup>, hoping to be regarded as a reliable chemical tool, or as “achieving full partnership with experiment as both an explanatory and predictive methodology” (Friesner, 2005, p. 6648). One can occasionally find suggestions that with the development of computers and quantum chemistry the time has come for organic chemists to give up using “familiar ball-and-stick and space-filling models and curly arrows in their explanations” (Veszprémi et. al., 1999, p. x). But other quantum chemists seem to aspire to the sort of insight provided by techniques like “pushing electrons” used by organic chemists, which is “very effective in rationalizing a large body of experimental results, and has good predictive power” (Jensen, 1999, p. xiv). It is worth considering whether, once one has factored out anxieties about the epistemological statuses of their disciplines, there is any real issue behind these divergent assessments of the prospects for quantum chemistry. I think that there is such an issue, but it is not a chemical issue so much as it is a philosophical one.

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<sup>3</sup> (Smit et. al., 1998, p. 456-7) assert that, “among our colleagues (mathematicians, physicists, and even physical chemists) there still pervades a bias that organic chemistry cannot be correctly listed as an exact science, but rather as the sum of empirical knowledge that has not yet undergone a sound quantitative treatment.” This conclusion is incorrect, they allege, because the exactness of organic chemistry “is not at all determined by the extent to which it uses the calculation methods of quantum chemistry” (Smit et. al., 1998, p. 456).

<sup>4</sup> (Jensen, 1999, p. xiv) claims: “The lack of quality assessment is probably one of the reasons why computational chemistry has (had) a somewhat bleak reputation. ‘If five different computational methods give five widely different results, what has computational chemistry contributed? You just pick the number closest to experiments and claim that you can reproduce experimental data accurately.’” Better, more informed quality assessment is one of the keys, Jensen claims, “to obtain results which are sufficiently accurate to provide useful information” (Jensen, 1999, p. 401)

Organic molecules are made of atoms, and atoms are composed of nuclei and electrons. Quantum mechanics is, from the point of view of 'fundamental' physics, the theory appropriate for characterizing the behavior of nuclei and electrons; thus in some sense quantum mechanics must be appropriate for characterizing the behavior of organic molecules. This much is agreed to by all parties. Disagreements arise when considering whether this conclusion leaves room for an autonomous, rigorous theory of organic chemistry that will not, eventually, even in principle, be swallowed up by quantum chemistry. It can seem puzzling that, or how, a theory could be appropriate for characterizing the behavior of organic molecules without somehow, in the limit of superfast computers, being replaceable by quantum mechanics.

Philosophically speaking, this issue is about the inference from an ontological premise, which chemists appear to share, to an epistemological conclusion—either the possibility or impossibility of an autonomous theory of organic chemistry. No chemists doubt that the organic molecules they consider, or even the macroscopic samples of such chemical that they work with in the lab, are composed of nuclei and electrons. Few doubt that the theory appropriate for describing the interactions of such particles, at least in isolated, individual contexts, is quantum mechanics. They disagree about whether these claims collectively entail that there will be some sort of epistemological reduction, in the limit, of the theory of organic chemistry to quantum mechanics. There is no dispute that as a matter of empirical fact, organic chemists are successful in solving problems appropriate to their field and that they do this, or are capable of doing this, largely without quantum chemistry. Further, few would argue, at least now, that quantum chemistry is sufficient for solving the significant problems of organic chemistry. So what is at stake is not the current autonomous status of the theory of organic chemistry, but rather the expectations for this theory going forward. Disagreements are about what to expect, and what to aim for, as organic chemistry continues to develop. Will, and should, the curly arrows and ball and stick representations of organic chemists eventually disappear, to be replaced by workstations and wavefunctions?

One aspect of this question has been extensively discussed in both the philosophical and chemical communities. This work has focused on the extent to which (or the sense in which) quantum chemistry reduces to quantum physics. Philosophers of chemistry, following the lead of some theoretical chemists themselves, have emphasized that there is no straightforward derivation of the approach taken in quantum chemistry (which assumes the independence of the nuclear and electronic

wavefunctions) from the principles of quantum mechanics<sup>5</sup>. Instead, fundamental chemical concepts like ‘structure’ and ‘bonds’ must be imposed on the pure formalism of quantum mechanics in order to make it applicable to chemical problems. This is a particular case of a more general observation: many of the successful ‘reductions’ trumpeted by scientists involve approximations, idealizations and/or empirical assumptions that cannot be rigorously, or straightforwardly, deduced from the reducing theory<sup>6</sup>. The philosophical implications of this observation are still in dispute and I will not pursue this point any further.

Instead, in this paper, I wish to consider a distinct question, which may make this prior question irrelevant, at least with respect to some of the general philosophical issues that drive reduction debates (such as the Unity of Science). I will consider whether, or in what sense, mainstream theoretical organic chemistry is reducible to quantum chemistry. This will not only open up a fresh perspective on the general issue of the extent to which chemistry and physics are unified, but also directly resonate with a live philosophical issue for chemists—should they anticipate the continued autonomy of theoretical organic chemistry? In order to approach this question, I will first try to characterize what it means to understand theoretical organic chemistry. Only by developing a relatively rich appreciation of what mastering this theory allows organic chemists to do can one then go on to ask whether a reducing theory, such as quantum chemistry, could ever hope to “accomplish the same purposes”<sup>7</sup> as theoretical organic chemistry.

What does understanding theoretical organic chemistry amount to? What can an accomplished organic chemist do with the curly arrows or ball-and-stick representations that are the tools of his or her theory? Without pretending to offer an exhaustive answer to this question, I will characterize understanding organic chemistry, for the purposes of this paper, as the ability to explain and predict some organic phenomena using the theory along with the ability to apply the theory in the solution of practical problems, such as designing the synthesis of a novel compound. This is in line with standard philosophical accounts of the role of scientific theories, except for the emphasis on application. In part, I think that

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<sup>5</sup> See (Weininger, 1984) for a summary of this issue from the point of view of a philosophically informed organic chemist. (Ramsey, 1997) presents this issue from a philosophical perspective.

<sup>6</sup> See (Sarkar, 2008, p. 431-3) on the general nature of this issue and its philosophical implications.

<sup>7</sup> See (Garfinkel, 1991, p. 443) for this quote and this general approach to issues of reduction.

philosophers have generally neglected the important interactions between theories and applications, but further, in the particular case of organic chemistry, it is essential to recognize the central place of synthesis in the discipline. Synthesis has been, by most accounts, the driving force behind the development of organic chemistry, but it makes demands of theory that are not well captured by traditional accounts of explanation and prediction. Additionally, it is hard to imagine better evidence for the power of a theoretical approach than the ability to manipulate and control the world evidenced by the successful total synthesis of a complex molecule<sup>8</sup>.

In order to characterize the understanding provided by both theoretical organic chemistry and quantum chemistry, I will employ some of the philosophical machinery developed by James Woodward in his manipulationist account of causal explanation (Woodward, 2003). Though I have some reservations about the details of his approach, the overall perspective that he takes on scientific theories and their role in scientific practice is useful in bringing out the differences between these two theories. Once these differences have been brought out, I will then argue that there are systematic reasons to suspect that quantum chemistry is incapable of supporting some significant explanations, predictions and applications that constitute an understanding of theoretical organic chemistry. The upshot, then, is that even should quantum chemistry be 'reducible to' quantum physics—in some suitable sense—there are good reasons to doubt that many of the significant results of theoretical organic chemistry could ever be reproduced by quantum chemistry alone.

## **1. What does Understanding a Scientific Theory Amount to?**

Woodward's approach to scientific explanation is distinctive in several ways that make it particularly useful for contrasting the theory of quantum chemistry and the theory of organic chemistry. First, Woodward focuses

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<sup>8</sup> See (Goodwin, 2008) for a detailed attempt to characterize how the theory of organic chemistry supports the manipulation and control of the world required by total synthesis. A version of this argument is made in (Smit et. al., 1998, pp. 458-9), where they claim: "Finally, as was stated many times by Woodward and other outstanding organic chemists, the successful accomplishment of a total synthesis is the best proof of the rigor and exactness of organic chemistry, since the multistep synthesis of a structurally complicated compound may be considered a viable undertaking only under the condition of a high predictability of the results in the whole sequence of reactions involved even when applied to previously unknown substrates."

on the sorts of explanations that scientists produce that are directly relevant to the manipulation and control of the world. Obviously, given the central role accorded to synthesis by organic chemists, one would expect the theory of organic chemistry to be well adapted to the goal of supporting manipulation and control. Woodward's approach is, therefore, particularly useful for bringing out how organic chemists can use their theory to plan and design novel syntheses. Additionally, one of the philosophically distinctive features of Woodward's approach is that it provides a common framework for thinking about explanation in both law-rich and law-poor disciplines. In other words, he characterizes scientific explanations in such a way that they may, or may not, appeal to Laws of Nature. Again, organic chemistry—though rich with explanatory generalizations that support manipulation and control—does not in the course of its theoretical work make many appeals to what are typically referred to as Laws of Nature. Quantum chemistry, by contrast, is largely concerned with approximating the results of applying the Schrodinger Equation—which might legitimately be called a Law of Nature—to particular cases of interest to chemists. Thus it is helpful to have a framework that transcends these differences when contrasting the role of theory in the scientific understanding supplied by these disciplines.

At the heart of Woodward's theory is the thought that scientific explanations are, for the most part, concerned with identifying interventions that might be made which would alter, in some respect or other, the phenomena. This is what distinguishes, on his view, explanations from descriptions. We can explain a result only when we understand what changes would have caused things to turn out differently; and this is an achievement over and above describing how things are. Explaining phenomena involves situating them within "systematic patterns of counterfactual dependence" (Woodward, 2003, p. 191). That is, we explain why something happened by bringing out the ways that the world might have been different so that the outcome would have changed in some specific sense. In order to do this, scientists must invoke claims about the possible ways that the world might be. Sometimes scientists do this by invoking Laws of Nature, which are typically regarded as describing necessary features of the world (or as characterizing relationships of broad scope that hold true no matter how the world might be). However, all that is really required, on Woodward's view, is an appeal to some sort of modally robust generalization. Such generalizations may be limited in scope, but so long as they imply that if certain changes were made, the world would have been different in certain specific ways, this is enough to support scientific explanations. Explanations are useful, from

this point of view, because in order to explain a phenomenon, one must be able to identify interventions that would, at least in principle, change the phenomenon some specific way. That is, one could predict how things would turn out differently if one were able to alter the conditions by such an intervention. Such predictions are at least part of what allows scientist to apply their knowledge in the solution of practical problems.

The changes in circumstances that are particularly important to a scientific discipline, according to Woodward, “help to set the explanatory agenda” (Woodward, 2003, p.262) for that field. This means that scientists concerned with changes of a particular sort seek modally robust generalizations that hold up across those changes; these are the generalizations that allow them to infer what would happen if such changes were to occur. As a result, “different choices of variables for theorizing are associated with different ways of carving up nature into possible alternatives, answers to different why-questions, and hence to different explanations” (Woodward, 2003, p.233). This means that on Woodward’s view, it is possible for there to be scientific disciplines that investigate the same objects, but which have distinct explanatory agendas with respect to those objects. Metaphorically, these disciplines would “carve up nature” into different pieces, according to the sorts of changes to which they were interested in subjecting those objects. In order to explain why their objects have certain characteristics (to answer Why-questions), these scientists must consider what changes; among the array of those that form their explanatory agenda, might modify those characteristics should they actually be implemented. This requires appeal to generalizations that hold up across some space of ways that the object might be changed. Scientists interested in different changes would, seemingly, require generalizations that differ in the space of alternatives that they span.

In the remainder of this paper, I will argue that the theory of organic chemistry and quantum chemistry are a case of this sort. That is, these theoretical approaches may have an object (or objects) in common—organic molecules—but they have different explanatory agendas with respect to these objects. As a result, the theoretical generalizations to which they appeal in explanations, predictions and applications are distinct. Organic molecules are, as it were, ‘carved-up’ differently in the two approaches and this is reflected in the fact that the space of alternatives into which they are situated differs. This does not imply that the two approaches are inconsistent, or otherwise unable to contribute to one another (which they clearly do), but it does suggest that there is something misguided about the thought that refinements in one of these theories would allow for total replacement of the other.



## 2. Understanding Theoretical Organic Chemistry

One way to get at the explanatory agenda of theoretical organic chemistry is to look at the sorts of Why-questions that organic chemists are interested in answering. Some attempts to characterize explanation in organic chemistry along these lines have been made (see Goodwin, 2003). According to this analysis, organic chemists are in large part interested in providing structural accounts of product distributions, relative rates, and some other related features of organic reactions (such as mechanistic pathways). Most of these explanations are contrastive, in that they take place against a backdrop of alternatives (the contrast class). For example, they might attempt to explain why a reaction is stereospecific rather than leading to a mix of stereoisomers, or why the dominant product is X rather than Y or Z, or why one reactant reacts so much more quickly than another. Certain kinds of differences between the alternatives in the contrast class are particularly salient for organic chemists, namely structural differences. So a satisfying explanation must identify what structural features of the molecules being considered are responsible for the contrastive fact being explained.

If this is a reasonable account of explanation in organic chemistry, then the space of alternatives into which particular phenomena are situated in this approach is a *space of alternative structures*. To explain why some contrastive fact is true about a particular molecule or reaction one would have to identify what structural feature might be changed so that that contrastive fact would no longer hold true. For example, if one explains that a particular reaction proceeds quickly, relative to some standard, because of neighboring-group effects, then this is to say that if the substrate were changed into a different structure that no longer had this neighboring group, it would no longer proceed as quickly relative to that standard. In order to support such a claim, one has to appeal to generalizations that hold up across some range of changes in structure. For instance, in this example, one might appeal to a claim like: “electron-releasing neighboring groups stabilize carbocations.” This is a generalization that is fairly robust across changes in both the structure of the neighboring-group and the structure of the cation, but it is not an exception-less law of nature. Still, it allows one to conclude that the reaction would probably not proceed as quickly if the neighboring group were replaced by a non-electron releasing substituent; and this is the kind of thing that a scientist must know, according to Woodward, if she is to explain, rather than just describe the phenomena she investigates. In virtue of knowing this, the organic chemist can make a range of specific

predictions about how an entire class of alternative substrates (all those that have different neighboring groups, but are otherwise similar) would behave. This predictive ability, in turn, supports the chemist's ability to manipulate and control organic reactions. To wit, it underwrites a maxim of the following form: If you want to (speed up/slow down) a reaction that proceeds through a carbocation intermediate, then consider manipulating the substrate by either (adding/removing) an electron-releasing neighboring group.

Thus far, I hope to have made it plausible that many of the explanations and predictions of organic chemists depend on generalizations about what structural features might be swapped out of an organic molecule in order to change its behavior in specific ways. I now want to try to make it plausible that these are the right sort of changes or alternatives for organic chemists to keep track of given some of their broader objectives. As suggested earlier, the novel synthesis of complex organic molecules has always been a 'center of significance' for organic chemists. This is just to say that one of the major ways that an achievement in organic chemistry can come to be seen as important is by either being, or contributing to, such novel syntheses. Accordingly, we should expect that the theory of organic chemistry is significant, at least in part<sup>9</sup>, because it supports the design of total syntheses of novel compounds. I have, in other work, tried to be explicit about how the theory of organic chemistry does this (Goodwin, 2009, 2008), but here I will have to be content with some suggestions.

One can think of synthetic design for a novel compound as the process of progressively pruning the 'retrosynthetic tree' of the target molecule<sup>10</sup>. The retrosynthetic tree of a compound is a branching collection of potential synthetic pathways, which is determined by the known synthetic transformations available to the designer. One can imagine generating such a tree by working backward from the target molecule in stages. In the first stage, one considers all the ways that one might generate the target molecule as the product of a known reaction and writes down the structures all of the reactants that would be needed to run these reactions. These structures are the nodes of the first stage. In subsequent stages, one considers all the ways that one might generate the nodes of the

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<sup>9</sup> In (Goodwin, 2008) I try to show how the theory of organic chemistry also supports both the implementation of a synthetic plan and the discovery of novel reactions.

<sup>10</sup> This way of talking is derived from the work of E. J. Corey (see Corey and Cheng, 1989), but I don't mean to suggest that it is original to him, or that his is the only, or best, way to think about synthetic design.

previous stage, and writes down a new array of nodes corresponding to the reactants for these reactions. The process continues until potential pathways end by generating nodes which one already knows how to synthesize. The generation of this array of potential synthetic routes requires using the taxonomic resources of structural organic chemistry. To generate the tree, one must be able to determine, based on the structure of an organic molecule, what (single-step) reactions might be used to make it. This requires not only the recognition of functional groups (or perhaps narrower structural patterns) in the molecule, but also a structurally characterized set of potential reactions (e.g. alcohols can be made by addition of water to an alkene). In this sense, the structural characterization of reactions and the functional group classification of molecules are conceptual resources required to even set up the problem of synthetic design. Once the problem is set up, the full theory of organic chemistry can be used to help make intelligent decisions about which of these routes are worth pursuing.

The selective exploration and evaluation of the retrosynthetic tree can be thought of, again following (Corey and Cheng, 1989), as occurring in three stages: strategic pruning, plausibility assessment, and optimization (for details see Goodwin, 2009). Each of these stages involves making assessments of what would happen should a previously known synthetic reaction be applied to a novel molecule. In order to do this, organic chemists need to know something about how that synthetic reaction occurs (its mechanism) and something about how the particular environment of the novel molecule will influence or modify the mechanism and/or reaction. Synthetic reactions are typically discovered, and their mechanisms investigated, in chemical structures substantially different from the novel molecules for which synthetic chemists must make these assessments. As a result, these chemists are required to evaluate how the characteristics of the known reaction would change should the structure of the substrate be modified in particular ways. In other words, they must evaluate the effects of swapping out parts of the standard structure (the structure on which the synthetic reaction was initially investigated) for the structural features relevant to the novel molecule that they are investigating. Doing this, in turn, requires appealing to generalizations that are robust across changes in structure, claims that span exactly the same space of possibilities as those employed in the explanations and predictions described in previous paragraphs. This is why the mastery of the theory of organic chemistry demonstrated in the explanations described earlier is useful in synthetic design, and therefore why the explanatory agenda of theoretical organic chemistry is *the space of*

*alternative structures*. The application of these generalizations in making assessments of the reactive possibilities of novel molecules is, however, often more complicated than it is in standard cases of explanation or prediction. Complex novel molecules often differ from reactive standard reactions in multiple overlapping, and possibly conflicting ways (they might have some features that promote a reaction and some that inhibit it). This typically puts them outside the empirically investigated scope of the generalizations that are being used in these assessments. The result is that these assessments rely on heuristics and make predictions that are often only contrastive (this will work better than that), qualitative (this is not likely to be stereospecific), or disjunctive (this is the range of possible results). Still, given the evident success of synthetic organic chemistry these theoretically grounded heuristics are an extremely effective tool for synthetic design.

To summarize, then, at least some of the significant results of organic chemistry depend on structural organic chemistry for their very formulation and on theoretical organic chemistry for the plausibility assessments that lead to their solution. These assessments require appeal to generalizations that span a range of ways that organic structures might be modified and this is at least part of the reason that the explanatory agenda of organic chemistry is focused on the *space of alternative structures*.

### 3. Explanation in Quantum Chemistry

Whereas we got a handle on the explanatory agenda of theoretical organic chemistry by characterizing the sorts of structural changes that were relevant to the field, it is easiest to characterize the explanatory agenda of quantum chemistry by looking at the sorts of generalizations or laws that figure in its explanations. According to Friesner (Friesner, 2005, p. 6648), the core technology of quantum chemistry is:

computational solution of the electronic Schrodinger equation; given the positions of a collection of atomic nuclei, and the total number of electrons in the system, calculate the electronic energy, electron density, and other properties by means of a well defined automated approximation.

This core technology has undergone marked development in recent years and as a result increasingly larger systems can be modeled to greater levels of detail and accuracy. The hope, at least according to Friesner, is that eventually “fully explanatory and predictive models” will be constructed for the “complex, condensed phase processes that govern most of the natural world” (Friesner, 2005, p. 6652). If we allow for the sake of

argument that Friesner is correct, and that quantum chemistry does indeed develop along the path that he envisions, it is still worth considering what kinds of explanations (i.e. which Why-questions) this technology will enable the chemist to provide, and which it won't.

Most fundamentally, the "core technology" of quantum chemistry can tell you the value of an output variable (the electronic energy or electron density, for example) when provided with a nuclear arrangement and an electron count. So far this is just a description, since from Woodward's perspective one must be able to say how things would be different after certain sorts of interventions in order to have an explanation. The sorts of interventions about which this core technology can provide direct information would seem to be limited by its input variables, namely the nuclear arrangement and electron count<sup>11</sup>. If this is right, then the quantum chemist can explain, for example, the electronic energy of a system in the sense that she can describe how that energy would change should the nuclear arrangement (or electron count) be altered. The space of possibilities across which the electronic Schrodinger equation ranges is therefore *the space of alternative nuclear arrangements* (and electron counts, perhaps). Keeping track of how the electronic energy or electronic density changes with changes in nuclear arrangements is very useful to chemists. Many features of individual molecules and chemical transformations can be reconstructed from such changes. For example, the equilibrium geometry of a molecule can be found by searching a subspace of the space of alternative nuclear arrangements corresponding to the range of different bond lengths and angles likely available to the molecule. The lowest energy nuclear arrangement in such a subspace would then correspond to the equilibrium geometry. Similarly, reactions can be explored by mapping how the electronic energy changes as the nuclear arrangement is shifted from that of the reactants to that of the products by a variety of different sequences of changes in nuclear arrangement. It is because of applications like (but not limited to) these, that quantum chemistry has been able to make increasingly important contributions to all areas of chemistry, including theoretical organic chemistry. Still, though this developing technology allows chemists to explain many things by keeping track of changes resulting from manipulations of the nuclear arrangement, there is no reason to think that every Why-question, or

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<sup>11</sup> When Woodward characterizes the explanations supported by an equation, or Law of Nature, he finds that additional interventions are supported by the argument pattern that leads to the equation. I am not sure how to generalize that in this case (Woodward, 2003, p. 190-192).

application, that chemists are interested in can be addressed by keeping track of such changes.

Most important, from the perspective of this paper, is that *the space of alternative nuclear arrangements* is distinct from *the space of alternative structures*. The array of distinct structures with which the organic chemist is professionally concerned differs from the target molecule not only in the arrangement of their nuclei, but also in the number and type of those nuclei. Consider, for instance, an organic chemist who explains why a solvolysis reaction runs on a substrate (say X) with an electron-releasing group (say -R) adjacent to the substituted carbon proceeds more quickly than the standard reaction without the neighboring group. The answer would likely appeal to the fact that reactions of this type proceed through a carbocation intermediate and therefore their transition states can be stabilized by a neighboring, electron-releasing group. This explanation has implications that go well beyond the particular structures (both X and R) that are actually mentioned in the original question. For one, by putting forward this explanation, the organic chemist implicitly suggests that it doesn't really matter which electron-releasing group is adjacent to the substituted carbon—any of them would be expected to have qualitatively similar effects. The structural difference that makes a difference, the organic chemist is saying, is that the adjacent group has a certain character (it is electron-releasing), and that character can be realized in a multiplicity of different ways. Furthermore, an explanation like this would typically imply a lot about the structural features that do not make a difference. For example, the particular structures considered might be acting as representatives of hydrocarbons with a good leaving group attached to a tertiary carbon (which would be the type of structure which undergoes solvolysis through a carbocation intermediate). If this were the case, then this particular explanation would be expected to be portable to (*ceteris paribus*) any other relevantly similar solvolysis reaction run on a structure in this broad class. It is the broad implications of an explanation like this that make establishing such an explanation useful to the organic chemist, for ultimately he or she will want to make reasonable assessments of how novel molecules will behave by invoking the principles behind such explanations.

By contrast, though the quantum chemist might be able to provide a detailed potential energy surface for the reaction in question (and even for the standard reaction to which it is being compared) from which the rate of the reaction can be derived (and shown to be higher than the standard), this does not by itself tell the chemist what structural features might be changed in order to modify the outcome. The potential energy surface

conveys how electronic energy changes with the nuclear arrangement, but it tells you nothing about what would happen to the rate if whole sections of molecule X were replaced by some other substituent (that would amount to shifting to an entirely different potential energy surface). To do that, you need generalizations that hold up across changes in structure, which is what organic chemists are in the business of providing. Without such generalizations, each structure is an island, which quantum chemistry may describe with mathematical precision, but which contains no clues about what to expect from other structures. As (Jensen, 1999, p. 347) puts it:

Although sophisticated electronic structure methods may be able to accurately predict a molecular structure or the outcome of a chemical reaction, the results are often hard to rationalize. It therefore becomes difficult to apply the findings to other similar systems.

Of course any particular question about how an alternative structure would behave could be answered by producing a new potential energy surface; but this is just more description without systematic attempts to uncover how rates and structures (or distinct potential energy surfaces) are related. These attempts might conceivably take a form different than the structural approach of modern organic chemistry (such as Frontier Molecular Orbital Theory or Marcus Theory, see Jensen, 1999, Chapter 15), but they would seem to require at least some form of theorizing over and above the core technology of quantum chemistry.

To reinforce this point, it is useful to try to imagine how a quantum chemist with a really fast computer but with no knowledge of organic chemistry might try to solve the problem of coming up with a plausible synthetic design for a complex, novel compound. Our chemist, let us imagine, is given a chemical structure, which amounts to a space of possible three dimensional arrangements of a set of particular nuclei and some fixed number of electrons. It is no problem to come up with an equilibrium geometry and even, perhaps, a set of possible molecular rearrangements corresponding to other minima on the potential energy surface. Solvent molecules might be added to develop a sense of the geometry in condensed phases. Before the process of synthetic design could even begin, however, the chemist would have to identify some set of chemical reactions that might be capable of producing the target molecule. By stipulation, this is a novel compound, so there is no history of past reactions having been run on the target molecule. Instead, somehow, a bunch of reactions run on different molecules are going to have to supply the array of possibilities for making the target molecule. It is hard to avoid

the conclusion that this will require some notion of *structural similarity* facilitating the application of past chemical experience to this new synthetic problem. Organic chemists have developed the concept of the functional group (and related structural classifications of reactions) to play this basic role, and it is not clear how our computer chemist could avoid something like it. Without some guidance from known organic chemistry, the quantum chemist would be at a loss as to which expanded potential energy surfaces in which to embed the target structure in order to evaluate potential reactions leading to its production.

Perhaps it is just too much to ask the computer chemist to come up with the retrosynthetic tree on her own, and instead, we could grant her the retrosynthetic tree and just ask her to do the pruning. But here, again, the computer chemist faces the difficulty that pruning the synthetic tree requires making assessments of how reactions run in very different circumstances will behave when applied in a new structural environment. Organic chemists approach these questions by characterizing the mechanisms of reactions and the effects of structural substitutions on those reactions, and this is frequently enough to make plausible assessments. Our quantum chemist, on the other hand, must approach the plausibility of each potential reaction in the retrosynthetic tree as a new, distinct question. After all, the particular relevant potential energy surface has never been mapped before. Quantum chemistry will not tell you which features of previously explored potential energy surfaces are likely to recur in the current case, at least not by using its core technology (it is interesting to note that computer programs designed to capture the logic of chemical synthesis are not built around the core technology of solving the electronic Schrodinger equation, instead they consist of heuristics for structural analysis, see Corey and Cheng, 1989). Furthermore, there would be no obvious guidance as to how much detail would be required in order to make realistic assessments of the plausibility of a reaction. For instance, solvents play a crucial role in many organic reactions, and so some reactions that are not synthetically useful in one solvent may be useful in another. Would each potential reaction therefore have to be evaluated on a range of potential energy surfaces reflecting the different solvents that might influence the synthetic plausibility of the reaction? At best, if organic chemists gave the quantum chemists the array of distinct potential energy surfaces worth investigating, the quantum chemists might, by brute force, be able to plow through these almost endless options and make some assessments of routes that might be synthetically plausible. To approach synthetic design in this way would, however, be the worst sort of purely empirical random groping. While she might be able to describe the



reactions that have accessible activation energies, she would have done nothing to embed these facts into the “systematic patterns of counterfactual dependence” that are the hallmark of a developed scientific understanding of a range of phenomena.

## Conclusion

In this paper, I argued that the theory of organic chemistry and quantum chemistry are theoretical approaches that have objects in common, but which have different explanatory agendas with respect to those objects. Whereas the theoretical generalizations of interest to organic chemists span *the space of alternative structures*, the core technology of quantum chemistry generates explanations spanning *the space of alternative nuclear arrangements*. These theories interact in useful ways, and they should generally be thought of as complements to one another rather than as competitors. I tried to show why it would be misguided to expect that eventually quantum chemistry would become the mathematical theory for the whole of chemistry. Synthetic design, which is where the theory of organic chemistry really comes into its own, requires generalizations that span *the space of alternative structures*. While the quantum chemist can be extremely useful in answering particular questions that come up in synthetic design, she is poorly equipped to generate and evaluate potential synthetic pathways, except in a brute and non-explanatory way.

This result is philosophically interesting for at least two reasons. First, the failure of quantum chemistry to support synthetic design is a clear example of how distinct sciences (or perhaps distinct levels of the same science) may ‘decompose’ the same objects or phenomena in different ways, and thereby support generalizations that are stable across different sorts of interventions. When the space of possibilities that are relevant to the significant problems of one science do not line up with those possibilities tracked in another science, then it is hard to see how the sciences could result in the same capacities to manipulate and control the world. Second, and more generally, this example demonstrates the fruits of considering the issue of Reduction not just in light of the explanations and predictions generated by a scientific theory, but also in the context of the applications—the potential for manipulation and control—facilitated by the theory. While the predictions and explanations generated by a theory typically play a central role in its justification, it is often the applications of a theory that are central to its significance. By focusing on what makes the truths generated by a field of inquiry valuable, and thus (in the case of

organic chemistry) on how the field confronts novel cases of application, new light is shed on the autonomy of the sciences.

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# METACHEMISTRY

## ALFRED NORDMANN

### Meta-Questions

Though it is hardly known or used at all, lacks a common definition, and sounds like a pun, the word “metachemistry” is no stranger than its well-established counterpart “metaphysics.”<sup>1</sup> Indeed, as soon as one begins to clarify the meaning or use of “metaphysics,” the need for something like metachemistry becomes readily apparent.

Metaphysics has nothing much to do with physics in a narrow, disciplinary sense, but it has everything to do with knowledge of the physical world, and thus with a kind of science of which physics is often taken to be the prime exemplar. If knowledge of the physical world consists in holding true beliefs about this world; metaphysics asks what the world must be like such that there can be knowledge of it. In the language of Kant, metaphysics concerns the conditions for the very possibility of an agreement between a representation and what it represents.<sup>2</sup> Accordingly, metaphysics has considered the notion of substance and those features of the world that persist through time—we can have knowledge about things if the world is such that at least some facts about it persist through time, otherwise we would have fleeting impressions only, but no beliefs that are true today and remain true. For that reason, metaphysics has also been concerned with the causal law or assumption of causality. If things happened spontaneously and without

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<sup>1</sup> An internet search in March 2012 produces a moderate number of hits for “metachemistry” but it is readily apparent that there are mostly incidental uses and no common definition. The more specific search “Bachelard metachemistry” leads to only a small number of hits, indicating that Bachelard’s neologism hasn’t caught on.

<sup>2</sup> As he set out to produce the first of his *Critiques*, Kant identified in a letter to Marcus Herz the question that “contains the key to the whole secret of hitherto still obscure metaphysics.” This question is: “What is the ground of the relation of that in us which we call representation to the object?” (Quoted in the introduction by Guyer and Wood to Kant 1997, pp. 47f.).

cause, we could not discern relations between events that are subject to representation. And thus metaphysics can be said to explore the many aspects of the “aboutness”-relation between knowledge claims and the world. And this relation, or so it is thought, absorbs much of epistemology and all of scientific knowledge: For theories, hypotheses, and other propositions to be true, they have to say something about something in such a way that there can be a lasting, non-accidental agreement between theory and reality, mind and world, the proposition and what it represents. All this may seem to be so obvious that it hardly requires stating—and with it comes the sense that metaphysics is an utterly familiar enterprise, no matter how confusing one may find it or worthy of critique.

While it may hold for physics that it seeks knowledge about the world and produces a theoretical representation of reality, this does not hold or holds only partly for chemistry. At the very least, chemistry serves as an example that the production of knowledge does not issue in theories only or even primarily, but that it issues also in compounds, industrial processes, testing routines and laboratory techniques. And instead of using predictions to test the agreement between representation and reality, the criterion of knowledge consists, for example, in the ability to move back and forth between synthesis and analysis.<sup>3</sup> So, rather than query the “aboutness”-relation between knowing subject and the world, it might be of equal interest to ask about the productive relation of knowing and doing and its conditions of possibility—about “working knowledge,” in other words: knowledge that is implicated in what works and that issues in pieces of work.<sup>4</sup> Here, for example, one might discuss Bachelard’s “realization of the real” (Bachelard 1968, pp. 47f.) or Peirce’s “reality as

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<sup>3</sup> It is worth entertaining as a thought experiment how much would be left of chemistry if it was stripped of words but consisted of routines e.g. to exhibit products in the back and forth between analytic and synthetic procedures. Indeed, quite a lot might be left, but whether it is a little or a lot, it would need to be reconstructed metachemically as a productive, non-representational kind of knowledge.

<sup>4</sup> Baird speaks of “working knowledge” in one chapter of his *Thing Knowledge*. This is closely related but not identical to the notion I am trying to articulate here, namely one of knowledge that is specifically acquired to make things work and that is exhibited and validated by the works (of art, of technology, of science or technoscience) that issue from it (2004, pp. 12, 48 and 66; Baird and Nordmann 1994). In search for the right expression I have tried “*Fertigkeitwissen*” (2011), “knowledge of control” (2012) and often refer to knowledge that consists in the acquisition and demonstration of (basic) capabilities (of control), including capabilities of manipulation, modeling, visualization. “Working knowledge” may turn out to be the most apt expression.

normal product of mental action” (1871, p. 91). Different from idealism or a constructivism that is opposed to realism, such explorations would aim to show that the world is reliable and robust due to the ways in which human agency is built into works of art, technology, or science, and inversely, that the world is built into human work.<sup>5</sup> Similarly, we might question the fundamental distinction of *physis* and *techné* and the many associated distinctions such as the ones between organism and artifact, nature and culture, cause and reason. These questions might lead to an understanding of powers and affordances, works and worlds that cuts across discovery and invention, what is found and what is made. Whereas—despite all their claims to novelty—process philosophy, dynamic conceptions of nature, or theories of self-organization merely propose alternative ways of properly representing reality, the attempts to articulate the preconditions and limits of working knowledge are metachemical.

This first approach at distinguishing metaphysics and metachemistry is perfectly general. Moreover, it might appear that many thinkers have taken steps towards metachemistry, even without calling it that.<sup>6</sup> So far, then, the term “metachemistry” has done little more than suggest that metaphysics revolves around representation, scientific experience, and the possibility of forging and securing some kind of agreement between mind and world.<sup>7</sup>

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<sup>5</sup> The work of Bruno Latour (e.g., 1999) comes to mind here but also that of Martin Heidegger (e.g., 1967) and others.

<sup>6</sup> I leave open here whether and where in the philosophical tradition one might find metachemical approaches already. While I am quite sure that process philosophy, theories of dynamic systems, self-organization, or emergence do not offer such an account, it might be more promising to look towards phenomenology or pragmatism. Charles Sanders Peirce, for example, compelling considers in tandem the production of knowledge and the production of reality, and he considers this not only as a human activity but as one of the universe. To read Peirce in this way requires severing his supposed affiliation with Popper and exhibiting his proximity e.g. to Latour (Nordmann 2009).

<sup>7</sup> To be sure, metaphysics does not imply a commitment to “representationalism” and to the idea that knowledge consists in the making of pictures. But the discussion of representationalism and its limits, and the many proposals of how to ground the possibility of agreement between mind and world in something other than likeness, all concern metaphysics. Likewise, metaphysical questions of “grounding the possibility of agreement between mind and world” do not imply a commitment to realism but might lead to idealist, positivist, or processualist positions, some of which will “anti-metaphysically” reject the metaphor of “grounding” and replace it with more positivist or empiricist accounts. These are the familiar debates in the tradition of metaphysics, broadly construed, yet limited to an interest in what the world must be like or how it must be conceived so that it can be known by the mind in the form of propositions and theories.

And once one appreciates this limited brief of metaphysics, there is room for the metachemical alternative and the attendant recognition that it is far less developed and that, in particular, we have no clear conception of working knowledge and thus of a kind of knowledge that is not about something and that is not true or false in virtue of how the world is. And if chemistry really does involve the production of such knowledge, we can see that the philosophy of chemistry is a place to look for contributions to the development of metachemistry.<sup>8</sup>

A chemically informed, otherwise programmatically metaphysical philosophy of science has contributed to this by way of Gaston Bachelard's *Philosophy of the "Non"* which introduced the term "metachemistry" (Bachelard 1968, 1981).<sup>9</sup> On very different grounds than Bachelard's, the philosophy of chemistry contributes now to the development of metachemistry, paradigmatically Bernadette Bensaude-Vincent and Johnathan Simon's *Chemistry—The Impure Science* (2008).

By looking in the following at Bensaude-Vincent and Simon's work first, one can see how it accords with the general characterization of metachemistry. And from this point of view, one can also see how this metachemical project picks up on Bachelard's conception and where it differs from it. This reframing of Bachelard's original project will bring to light that the different questions of metaphysics and metachemistry arise not from the disciplinary juxtaposition of physics and chemistry. Instead, they arise from the juxtaposition of physics as a science and chemistry as a technoscience—where technoscience is nothing more or less than research that does not produce knowledge *about* the world but produces working knowledge. Negatively defined, technoscience is impure in that it abandons the work of separating representations from what they represent, of separation the work of technology or culture from the work of science or nature. Positively defined, technoscientific research takes place in a technological setting and in a technological manner in that it develops and achieves basic capabilities for controlling processes and phenomena, even

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<sup>8</sup> Again, the philosophy of chemistry cannot possibly be canvassed here. Papers like Newman 1989, Schummer 2003, or Bernal and Daza 2010 come to mind, and of course, the work to be discussed further along in this paper.

<sup>9</sup> The title of Bachelard's book was translated *Philosophy of No* but this is misleading in that Bachelard refers to non-Aristotelian logic, non-Euclidean geometry, or non-Lavoisian chemistry—where the "non" signifies not outright negation but a next stage in the development of science, namely a stage that in Hegelian fashion sublimates (overcomes and includes) the previous stages. Accordingly, Bachelard speaks of non-Lavoisian chemistry as "dialectizing" and differentiating the conception of substance in Lavoisian chemistry (1981, 59).

where that control might consist in the ability to exhibit surprising things—and thus, technoscience is defined as the kind of research that requires not metaphysics but metachemistry.<sup>10</sup> So, while at first it might appear to be a subtle point that metaphysics and metachemistry do not owe to the difference between physics and chemistry but to the difference between physics as science and chemistry as technoscience, this point involves quite a lot—in particular, a genuine appreciation of impurity and of chemistry as an impure (techno)science.<sup>11</sup>

## Pure and Impure

Metaphysics is all about purity, and from a metaphysical point of view the apparent impurity of chemistry is a blemish that needs to be cleared up. This concern with purity comes with the turf if one wants to account for the aboutness-relation: In order to understand how a representation can agree with what it represents or how a proposition is true of some state of affairs, things need to be held apart before they can be related to one another. Since scientific vocabularies and technical procedures usually define the objects of study, one needs to determine as precisely as possible what concepts, representational devices and experimental techniques do, and at what point they are confronted with mind-independent features of the world—features that can warrant agreement of theory and reality. Especially with the tradition of Kantianism, a lot of effort has gone into specifications of empirical content, such efforts have established an ideal of pure science which has proven enormously influential even though it is continuously under threat of being exposed or debunked.<sup>12</sup>

For the most part the philosophy of chemistry has inherited this metaphysical brief when it seeks to define a specifically, purely chemical manner of representing specifically, purely chemical objects or processes. This concern for the disciplinary identity of chemistry aims to remove the blemish of impurity especially in regard to physics and the notion that the better part of chemistry is physics and the rest a kind of ill-understood,

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<sup>10</sup> For this definition of technoscience and its precursors see Bensaude-Vincent et al. 2011 and her paper within this volume.

<sup>11</sup> Indeed, the point can be pushed further by taking the case back to physics: The different questions of metaphysics and metachemistry arise from the juxtaposition of physics as a science and physics as a technoscience—as soon as one begins to appreciate the impurity of physics as craft or technology.

<sup>12</sup> We owe to Michael Friedman the recognition of the pervasiveness of the Kantian tradition in canonical philosophy of science (e.g., Friedman 2001).



application-oriented craft.<sup>13</sup> Indeed, much of the philosophy of chemistry is informed by the suspicion that chemistry as we see it today is not real chemistry but a kind of physics. And even those who think that today's chemistry is real chemistry are prone to query what aspects of contemporary chemical research are beholden to physics, where chemistry becomes chemical, and how it is that chemistry is by no means inferior to physics. Rather than take their problems from the discipline as they find it, they therefore tend to remind chemists of who they are or who they ought to be. In particular, many philosophers of chemistry shift attention from immutable physical processes at the atomic and molecular levels to chemistry as an art of transmutation, that is, of changing one kind of physical stuff into another. Accordingly, philosophers of chemistry often contradict the "official" story of modern chemistry's separation from alchemy as a feat that was accomplished for good by its founding father Lavoisier. Instead, they tend to take seriously the alchemical origins of chemistry and carefully account for the vestiges of alchemical thinking.

In *Chemistry: The Impure Science* Bernadette Bensaude-Vincent and Jonathan Simon depart from this tradition in the philosophy of chemistry by offering a far more radical proposal. They want to save chemistry not from physics but from metaphysics, that is, from the concern to establish the peculiar dignity and purity of chemistry. Rather than establish its disciplinary identity in the concert of scientific disciplines, Bensaude-Vincent and Simon treat chemistry as an eclectic ensemble of ideas and practices. If it is defined at all, this impure science is defined by its technoscientific ambitions, which provide a common bond that extends from alchemy all the way to nanotechnology.<sup>14</sup> Instead of beginning with chemical substance, with elements and compounds, with analysis and synthesis, with reaction, process, and complexity, the book therefore begins right in the middle with DDT and Bakelite, with impurities that include environmental pollution and the transgression of traditional divisions between nature and artifact, science and technology. And yet, its argument for chemistry as an impure science does not rely on fashionable notions of hybridity. What puts chemists in the midst of things is their predicament of being "condemned to stumbling their way through the darkness, trapped at the level of phenomena and never having access to the underlying substantial reality, knowing only the outcomes and not the reasons" (2008, 62). This predicament, however, is not to the detriment of

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<sup>13</sup> The remainder of this and the following two paragraphs are incorporated from a review of Bensaude-Vincent and Simon's book in Nordmann 2010.

<sup>14</sup> Perhaps, the final punchline of this book can be put as follows: Nanotechnology shows that chemistry never ceased to be alchemy.

chemistry. Whether at the phenomenological level of observing chemical reactions or at an analytic level of instrumentally engaging with molecular structure, chemists always encounter matter in its material aspects, that is, superficially. Their different ways of experiencing and dealing with chemical matter treat atoms, molecules, and macroscopic samples on the same plane ontologically — there is not one reality behind the other, there is nothing underlying or hidden or true beneath the phenomenological, superficial, or illusory (2008, 145, 204). Accordingly, the standard metaphysical question of positivism versus realism fails to gain traction (2008, 199): On the one hand, chemists claim a positivistic attitude that sticks to sense data and does not infer a true reality behind the appearances, on the other hand they work with valences and bonds, with atoms and molecules in a manner that takes these to be unquestionably real. Similarly, the metaphysical question of reductionism is not germane to chemistry. The question presupposes that the levels between which chemists move with great facility can be held apart and queried for their relations. It thereby presupposes also that chemistry and physics can be considered as distinct even while chemistry appropriates so much of physics.

One might now be tempted to consider what Bensaude-Vincent and Simon call the chemists' "operational realism" as a metaphysical stance of its own which involves a theory of matter that defies classical categories. But again, they insist that this is not an alternative metaphysics (2008, 143–145), in part because chemists are not sufficiently interested in clarity and distinctness, and do not hold consistency to be a very high value (2008, 3). For example, the problem of the mixt has never been resolved or displaced by the notion of a compound, corpuscularism still haunts atomism, elements coexist with principles, and the periodic table remains both a practical toolbox and a foundational system (2008, 124–126, 135–138, 160, 170–172). Chemistry's challenge to philosophy is therefore not that it requires better rational reconstructions of its implicit metaphysics so as to hold it distinct from physics and biology. Rather, the challenge is to appreciate that the elements of the periodic table are analytic objects for conceptual manipulation and at the same time empirical objects for material manipulation (2008, 192). Or, to put it differently, the challenge is to see that even without a theory of matter, chemists develop notions of matter that allow them to interpret reality (2008, 145)—that they do theoretical work even as they eschew consistency and do not refer appearances to true underlying realities. From the midst of the mixt, so to speak, Bensaude-Vincent and Simon call for a philosophy of science that abandons its interest in purifying the impure science of

chemistry by using metaphysics as an instrument for the clarification of principles, concepts, and commitments.

To be sure, the rejection of the metaphysical brief is not enough. In the end, an account is needed of just how chemists do theoretical work without applying theories, and how they can interpret reality through conceptions of matter that are implicit in their practice and do not amount to representations of what matter, or of what chemical reality is. Here Bensaude-Vincent and Simon's account is tantalizing sketchy and merely suggestive. And here, it is fruitful to look back at Gaston Bachelard's *Philosophy of the Non*.

### Bachelard's Metachemistry

Bensaude-Vincent and Simon refuse to consider chemistry metaphysically and take seriously its character as an impure science or technoscience. From their point of view, the impurity of chemistry, its ontological indifference (Galison 2006, also Daston and Galison 2007, p. 393, 414) and lack of concern with the structure of reality is an asset and not a blemish. It underwrites chemistry's productivity of compounds, materials, procedures, techniques, and models. Metaphysical questions of realism versus constructivism do not gain traction and can neither impeach nor underwrite chemical knowledge. But for all these evidences of their metachemical orientation,<sup>15</sup> Bensaude-Vincent and Simon do not invoke "metachemistry" to designate their project. Indeed, they explicitly deny that they are continuing "Bachelard's project of constructing a metachemistry as the chemical counterpart to metaphysics" (Bensaude-Vincent and Simon 2010, 382). The reason for this is obvious enough. In contrast to metachemistry as introduced quite generally above, Bachelard proposes the term in order to articulate the significance of an emerging new science that creates in its wake also a new philosophy (1984, 3). He pursues a "presentiment of a profound revolution in chemical philosophy," and as part of this imminent revolution, "metachemistry would already seem to be a possibility" (1981, 53). Through a succession of epistemic breaks, each saying "no" to a conception of substance that came before it, contemporary mid-20<sup>th</sup> century chemistry finally allows for a metachemical conception of substance. And thus, Bachelard's "metachemistry" marks a

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<sup>15</sup> More evidences could be added, especially as they describe physics as adhering to a deductivist project of representation, whereas chemistry is viewed technoscientifically not as providing a picture of reality or theoretical understanding, but as a manner of working with materials and other tools to produce new materials.

clean break with the past and serves in his historical reconstruction to purify one notion of substance, and one idea of chemistry in contradistinction to others. Quite evidently, this entire program and philosophy of scientific history is caught up in a metaphysical concern with successive modes of representation, and it runs counter to Bensaude-Vincent and Simon's conception of chemistry as an impure technoscience that represents a tradition of practice that ranges at least from alchemy to nanotechnology.<sup>16</sup> And thus, when Bachelard writes that "[m]etachemistry would be to metaphysics in the same relation as chemistry to physics" (1968, 45; 1981, 53), he operates, despite himself, with a metaphysical conception of chemistry as a discipline *sui generis*, namely a discipline characterized by a distinctive mode of representing its objects.

But even if one agrees with the rejection of Bachelard's program, his conception of metachemistry is still fruitful and was meant by Bachelard to provide insight beyond a particular epoch in the history of science. Like many dialectical thinkers and also like contemporary philosophers of technoscience, he explores a contemporary state of development only to discover that it serves to describe all of history.<sup>17</sup> The metachemical conception of substance, in particular, allows one to conceive the entire succession of conceptions of substance as a trajectory that, in effect, dissolves the very notion of substance as something persistent that might

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<sup>16</sup> "This leads us to reject the quest for metachemistry and instead to pose the question: to what extent can our epistemological, ontological and anthropological characterization of chemistry be extended to the entire realm of contemporary practices in the natural sciences?" Bensaude-Vincent and Simon identify another pertinent limitation of Bachelard's thinking: "By emphasizing the technological component of chemistry, he promoted this science as a model for a new philosophy of science, a rational materialism based on phenomenotechnics. However, the technological dimension of science in Bachelard's works is confined to his views of an instrument as a 'reified theorem' and chemical synthesis as the concrete expression of a human project" (2010, 382).—As opposed to Bensaude-Vincent and Simon, Bachelard wants to strictly distinguish chemistry from alchemy even though, arguably, his notion of the „realization of the real“ applies equally well to chemistry and to alchemical routines of purifying and transmuting material stuff as well as the souls of the alchemists.

<sup>17</sup> Donna Haraway, Bruno Latour, or Andrew Pickering discovered technoscience as a contemporary hybrid of science and technology ("these can no longer be distinguished") and went on to say that there was never a pure science anyhow, and that all previous attempts to juxtapose science and technology were ideological ("there was never a proper distinction"). This universalizing move has been criticized by Rabinow 1997.—Along similar lines, Bachelard can be found claiming Mendeleef's tables as the birthplace of metachemistry (1981, 58).

serve as an object of representation. The ultimate substance of ‘substance’ is its own history of rationalizations and conceptualizations and their associated practices (1968, 44, 72f., 76).

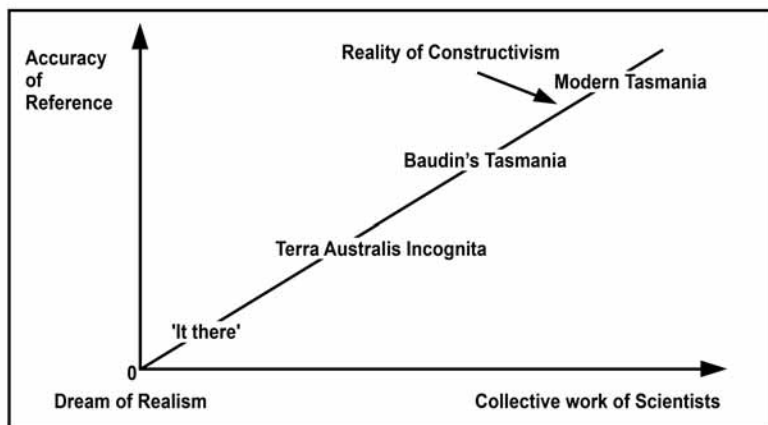
Metaphysics could have only one possible notion of substance because the elementary conception of physical phenomena was content to study a geometrical solid characterized by general properties. Metachemistry will benefit by the chemical knowledge of various substantial activities. It will also benefit by the fact that true chemical substances are the products of technique rather than bodies found in reality. This is as much as to show that the real in chemistry is a realization. (1968, 45)

When Bachelard speaks of “[c]hemical knowledge of various substantial activities” this conception includes the above-mentioned working knowledge of techniques, which can participate in material agencies so as to afford substances as works of chemistry. That the real is a realization (rather than, say, a discovery or a construction) appears to be a general point about the technosciences which do not seek primarily to represent and understand the world but which, impurely, combine various productive agencies. Here, Bachelard’s notion of metachemistry agrees with the general meaning assigned to it above. Substance conceived metaphysically refers to the persistence or obduracy of features of a mind-independent reality—it is a subject of representation only if the propositions about those features say something that is not already known. This ‘substance’ is introduced as an unknown, at least as yet unknown nature of things that persists so that we can gain knowledge of it. “[F]or a chemist who has just realized a synthesis, chemical substance must, on the contrary, be equated with what one knows about it” (1968, 47) and, in particular, what is known in the process of making. If chemical substance is thus tied to knowledge, it is not a definite something or mere substrate that endures through time. Instead, it is at all times fully realized as just what it appears to be, and at the same time it never stays the same as it becomes transformed in processes of making, remaking, and learning to make. As an indefinite “something out there”—like a material probe for chemical analysis or an apparent disorder presented at a clinic—the substance enters into a series of interactions that produce determinate things that are characterized by their performance, functionality, or affordances. That substance is always no more and no less than what we know about the techniques of exhibiting it, underwrites Bachelard’s curiously rationalistic story of successive epistemic breaks but agrees also with Bensaude-Vincent and Simon’s picture of chemistry as treating all modes of chemical experience on the same plane.

Bachelard describes the trajectory of successive states of knowledge or competence in terms that were later echoed by Bruno Latour (Nordmann 2006). This trajectory becomes visible “when one of the variables included in the representation is *time* and the other variable corresponds to some characteristic of substance” (1968, 64). In this kind of graph, Bachelard suggests, one can plot the definition or institution of substance. The choice of variables avoids the metaphysical presupposition that there is a stable “it” that is being represented with ever greater accuracy: the probe and the disorder are perfectly well-known and can be described in great detail before chemical composition is revealed or a specific disease defined. The apparent constancy of this “it” emerges only from a continuity of interaction and its narrative order—it is the story of interactions that build upon one another and accrue competences or knowledge to produce behavioral performances that fix a common referent that has always been there (Latour 1996, Latour 1999, pp. 145-173). In the context of this storyline, substances result from the accumulation of more and more characteristics: They appear to become more articulate and better articulated as they incorporate “more and more of the conditions needed to detect them” (1968, 59). Considered along the continuous path of this trajectory, substances become increasingly reliable or stable actors in experimental and technological interactions, that is, as the situations are defined and become defined in which they will assert themselves in certain ways. The trajectory is therefore graphed in reference to two variables: The time that passes as the collective work of science goes on, and a scale that registers the accumulation of characteristics with which the substance becomes identified. 50 years later, the graph envisioned by Bachelard was actually produced by Bruno Latour with respect to Pasteur’s experiments and the “discovery” of Tasmania (1990).<sup>18</sup>

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<sup>18</sup> To be sure, the graph that here appears to be co-produced by Bachelard and Latour brings out a tension in Bachelard’s account: The graph highlights the continuity of a process through which some “it” becomes ever more definite and through which the real is determined, that is, the continuous accumulation of characteristics (this continuity also accords with Peirce’s philosophy). Bachelard, of course, is also likely to point out the discontinuity of epistemic breaks—and he is thereby closer to Bensaude-Vincent and Simon’s account that implicitly rejects the teleology of a continuous trajectory of realization.



Despite its curiously Hegelian notion of an advancement of thinking about substance that has reached a particular stage during the first half of the 20<sup>th</sup> century, Bachelard's historicist and technological understanding of substance as substance-in-the-making thus meets up with the perfectly general account of Bruno Latour. Accordingly, Bachelard's idiosyncratic notion of metachemistry offers one avenue towards making more precise the general and vague conception at the opening of this chapter.

## Working Knowledge

On the basis of these rather principled and conceptual considerations, we can finally turn to technoscientific practices that call for metachemical reconstructions. For each of these practices one should ask what specific relation they forge between knowing and making. So far, chemistry came in through the work of Bensaude-Vincent and Simon as a prominent exemplar of an impure technoscience. Also, chemistry came into play with Bachelard's contrast of physical or metaphysical substance (a geometrical solid characterized by general properties) and chemical or metachemical substance (the material stuff that enters the laboratory and through constant reworking becomes a product that affords particular interactions). When we here go on to cite examples of technoscientific practice that call for metachemical reconstructions, chemistry appears as before now and there—prominent but by no means privileged.

Of the following examples of technoscientific method, the one that is most intimately tied to the relation of knowing and making is the demand that chemical analysis needs to be matched by synthesis. This demand, in

turn, is emblematic of the entire tradition of Baconian science (Smith 2004, 239) and it has just recently attracted attention in the field of Synthetic Biology with its frequent invocation of Richard Feynman's dictum "What I cannot create, I do not understand" which seems closely related at first sight to "what I cannot synthesize, I have not analyzed." In all likelihood, however, this dictum takes on a different meaning when it moves from the blackboard of a physicist who is committed to a scientific ideal of theoretical understanding to a research community that prizes making and building. It needs to be appreciated in respect to the metaphysical conceptions that can underwrite agreement theory and reality and in respect to the metachemical conceptions that can underwrite the participation of human agency in material agency. In particular, does Feynman's dictum provide a necessary condition for understanding, for successful and complete analysis—where the ability to create or synthesize is conclusive evidence that validates a theory or proposed analysis? On this interpretation, understanding is intellectual and consists in a representation or mental model of a phenomenon, and the ability to create confirms the mental model. While this is probably what Feynman meant to say, at least some proponents of Synthetic Biology take his statement as providing a sufficient condition "what I create, I thereby also understand" (again, see Benner and Sismour 2005). This reading is unintelligible and must be rejected as long as understanding is tied to the aboutness-relation and as long as it concerns the relation of mind and world. On a metachemical reconstruction it might become intelligible—if, for example, the ability to create is taken as a form of successful participation in the world, a sign of having achieved a feeling for the behavior of a physical system.<sup>19</sup>

If the realization of the real involves participation in the real, the separation of mind and world as separate spheres is no longer possible—and with that, there is also no separation between the superficiality of mere appearances and the depth of explanatory structures behind the appearances. And thus, we are back in the midst Bensaude-Vincent and Simon's account and in the midst of the impure where metaphysical debates about foundationalism, reductionism, positivism vs. realism do not gain traction. This holds also for questions of compositionality—is water made up of the two components hydrogen and oxygen, or is there salt in

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<sup>19</sup> Feynman's statement has also been understood as a modern formulation of Giambattista Vico's *verum factum* principle which places a limit on the ability to understand nature as something that humans have not created and therefore will never properly understand (Schummer 2011, 136-147).



the sea?<sup>20</sup> As before, this question requires different treatment in the context of seeking to know the world representationally by way of true propositions, and in the context of knowing the world technologically in the course of acquiring capabilities of control. That the whole might be more than the sum of its parts and similar notions are necessary metaphysical devices to represent systems and a special class of properties that are now called emergent. At the same time, mereological notions of components and systems can be considered grammars of chemical practice that regulate the movement of researchers between atoms and elements, molecules and bulk matter, and the devices that address and interact with them. Molecules do not “emerge” from atoms, and certainly they do not “self-organize.” Instead a certain organization of technical attention, one that includes mereological conceptions but also laboratory apparatus and physical samples, affords molecules or affords atoms or even affords commonplace bulk matter: “There is no sodium in salt, but salt affords sodium” (Harré and Llored, 2011, 70). Mereology (and similarly, causality) as a grammar for interaction with the world is always implicated in the relation of making and knowing. When technoscientists in their laboratory show that this process yields that outcome or that they can reliably produce a surprising effect or that in this probe they can isolate that trace element, these capabilities involve par excellence an implicit or explicit conception of parts and wholes, constituents and components, structures and functions, of bits as distinct from parts, of fusions as distinct from sums. A similar point can be made in regard to causality: implicit knowledge of what kinds of actions are necessary and jointly sufficient to produce a certain kind of effect involves a conception of the ways in which the work of people upon material stuff is productive and affords works of art, of engineering, or of technoscience.

To be sure, a lot of further detail is required here: Technoscientific working knowledge participates in the world by way of producing works that afford activities and things (Harré 2003). This sets it apart from a magical mode of participation that seeks to change the world through the manipulation of signs. A voodoo doll that is in some ways similar to a human being if only, say, by sharing a lock of hair with that person, does not represent or symbolize her. Instead, it is an icon that shares in the reality of that person such that actions on the doll are simultaneously actions towards that person. In contrast, working knowledge participates in the world through the technological creation of works, as, for example, in

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<sup>20</sup> The following remarks are inspired but do not begin to do justice to Harré and Llored (2011).

alchemy, chemistry, and nanotechnology. Here too, this involves the creation of iconic devices that share in the reality of something else. One such device would be a so-called CAVE-environment that allows researchers to interact “face to face” with molecules, which includes not only to see but even to feel molecules as molecules “see” or “feel” each other. This is accomplished by entering a cave-like three-dimensional simulation model and by experimentally intervening in a scaled-up molecular world by pushing and pulling and thus experiencing binding forces first-hand in this substitute environment. Since the CAVE has many features of reality packed into it (not unlike that lock of hair), action performed in its environments are thought to be actions on the “real” physical entities (which is how one can speak of simulation *experiments*).<sup>21</sup> And as in pre-modern magical thinking (Foucault 1973), the mere likeness or similarity of two things suffices to infer a common cause—since an experimentally obtained and a calculated image look alike, one infers that they owe to the same causal dynamic, even if this dynamic is implemented in the computer in one case and an experimental system, in the other case. That the similarity of things should testify to their participation in a shared reality and that this should underwrite causal inferences is difficult, if not impossible to reconstruct with classical epistemology that seeks to avoid circularity by ensuring that evidence is independent from and external to theories and their models. As opposed to voodoo, however, causal inferences from a CAVE environment or from a genetically engineered animal model for a human disease are by no means unfounded. They are underwritten by the technical construction of the substitute reality and all the theoretical as well as working knowledge that goes into it (Reinhardt 2006).

To conclude this cursory list of research practices that call for a metachemical conception of knowing and making in the world, here is an immersive routine of working knowledge that produces participation in a system through a process of taking on ever more features of the world such that it can finally serve as a substitute for it. This is the routine that Hasok Chang has identified for the construction of measuring instruments and that is now being explicitly transferred from software engineering to the construction of synthetic organisms (Chang 2004, O'Malley 2009).<sup>22</sup>

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<sup>21</sup> This point can be extended to many simulation models, animal models, and generally „models for“ in contrast to „models of“ (Fox Keller 2000).

<sup>22</sup> Chang takes Peirce's epistemology of self-correction as a model for this process of iteration. But rather than tending to the limit of a frequency, the iterative self-corrections of measuring devices resemble the technological model from software engineering.

The iterative loop looks simple enough. It begins with an analysis that is used to construct a model that then exhibits some behavior. Here the second cycle begins with an analysis of the behavior of the model that informs the correction of the model that then exhibits a somewhat different behavior. And thus commences a process of tuning a model to exhibit a desired behavior which is similar, perhaps, to a complex behavioral pattern that is observed in the “real” world. By incorporating more and more knowledge of that world into the corrections of the model, the model gains in complexity and participates ever more deeply in the workings of the world.<sup>23</sup> This iterative process thus began with an aboutness-relation and a classic notion of representation but moved on to produce a working knowledge that has become reliable due to a process of assimilation: The researchers began with an analysis of a process or phenomenon, event or situation that led to the construction of an initial model that represented the situation in question. But with each subsequent iteration they absorb more and more of the world into the model—they no longer analyze the situation in order to speak about the world, but they analyze the behavior of the mode in order to imitate the world. The researchers thus gain a feeling for the behavior of the complex system that is growing up under their hands, and they lose analytic or theoretical understanding in the form of intellectually tractable claims about the world (cf. Lenhard 2011). Their realization of the real follows a metachemical trajectory: they gradually incorporate more and more of the world into their works and thereby learn to know it. And thus, if metaphysics is concerned with what the world must be like in order to support aboutness-relations, the task of metachemistry is to explore how the working knowledge of researchers affords works of technoscience that share in the same reality as the works of nature, and moreover, to explore the significance of the participation of works in the world and of the world in the work of technoscience.

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<sup>23</sup> This is an instance also of what Andrew Pickering calls *the mangle of practice* (1995)—attempting to differentiate and specify what is glossed over and lumped together by the notion of the “mangle.”

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# GLOBAL CONCLUSION: INVESTIGATING THE INTERPLAY BETWEEN CHEMISTRY, CHEMICAL PRACTICE, AND PHILOSOPHY

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The practitioners of “green” chemistry and of nanochemistry as well as the great names of earlier quantum chemistry, to cite but a few examples, do not form homogeneous communities. Like the chemists of the emerging organic field of research during the 19<sup>th</sup> century, they encompassed multifarious ways of doing chemistry. In addition to the various ‘communities’ of chemists there were sources of both knowledge and know-how coming from many other domains of sciences, and, sometimes, from society. Ana Simões and Kostas Gavroglu clearly point out this diversity as regards quantum chemistry. In the same vein, other studies within this volume demonstrate that green chemistry is not a delineated field. The term “green chemistry” does not have a unique reference. A chemist who optimizes an extraction process using a supercritical fluid does not make use of the same chemical practice as does a specialist in molecular assembly using transition metals. They are both chemists and mostly use the same molecular representations, but they do not have the same chemical culture and know-how. Moreover, they do not use the same *resources* in the same *sites* with the same *aims*: their scientific “forms of life” and “styles of work” differ.

It is not solely *the conjunction but, above all, the mutual interferences between those forms of life and the translations from one to another* that are subsumed under the label “green chemistry”. Moreover, those forms of chemical life themselves are at stake within current research programmes. This volume thus strengthens an image of chemistry constantly adopting new techniques and concepts and pushing on the frontiers of neighbouring fields of science.

In her book, *The Invention of Modern Science*, Isabelle Stengers asserts that science is a process rather than a product; it is creative rather than

foundational; it creates truths rather than “The Truth”. Its action introduces novelty into the world; it “makes a difference”. She upholds the view that a scrutiny of a scientific “event” is basic for grasping scientific novelty and evolution, without accepting ready-made philosophical dichotomies such as theory and observation, fact and law, and so on. We thus have to “follow the process” in so far as the process is precisely what is at issue (Stengers, 2000). It is important, first of all, to scrutinize what is happening in actual laboratories, as well as the procedures followed there. In this respect, studying chemistry philosophically requires the integration of chemists’ own questioning into the global pattern of the investigation of nature. This is what this volume genuinely achieves. In doing so, it fills a gap in the philosophy of science, in so far as it closely associates chemists from various domains to the epistemological and philosophical investigations that are relevant to them. In so doing, it integrates chemical practices into the philosophical adventure in a manner different from the tradition; that is to say, by means of collaborations between chemists, historians, and philosophers. We begin by examining what chemists are doing mainly in order to: (1) investigate chemistry, (2) think about methodologies, and finally (3) create or reshape concepts. In doing so, we highlight how chemistry is changing in relation with other human domains. This road leads us to query how new chemical practices emerge and how they are reinterpreted by the chemists themselves. We then stress how this study is important for philosophers in order to think about science.

In his *Brown Book*, Wittgenstein shows that there is no sharp boundary around a generic term (Wittgenstein, 1969). Its unity is thus the result not of a strict identity or of a unique reference but, on the contrary, of a network of overlapping resemblances, none of which run through the totality. “Similarities” imply subtle “differences”, not identity, direct foundation, or reference. We are dealing here with differences *in kind*; a family resemblance is not an open door to an infinite conjunction under the same denomination. Grouping incompatible rules of grammar and empirical propositions under the same label leads to a category mistake. The labels ‘sustainable chemistry’, ‘green chemistry’, and others all refer to their own background with their own practices, goals, representations, know-how, and resources. Family resemblance makes the coexistence of different meanings and their interaction possible depending on the *contexts* of use and what chemists aim at doing. Family resemblance may afford a “coherent pluralism” at a particular time, to use Bachelard’s turn of phrase (Bachelard, 1932). This pluralism implements the narrative reconstruction



that chemists develop *a posteriori* regarding their own activities, in order to build a community identity and to gain legitimacy.

Assigning new meanings, new roles within hierarchies, and new relevant goals and methods to the different protagonists and institutions that are involved in the process of innovation is a “political” task. There is nothing transcendent in this story, no real primary “frontier” between the inside and the outside of a particular chemical domain. There is only an “immanent process of deterritorializations and reterritorializations”, to use Deleuze and Guattari’s terminology (Deleuze and Guattari, 1987). Bachelard has already declared that “[e]ach interesting problem, each experiment, or even each equation required a philosophical reflection of its own” (Bachelard, 1940, 1968). Without the multiplication of perspectives, there is no objectivity! The study of details is, therefore, of primary importance. To achieve this, we need each and every kind of expertise. In this respect, instead of opposing alleged philosophical ‘traditions’, philosophers should delineate a problem, for example, the study of the ontological status of chemistry. They should envisage how the different approaches provide them with complementary perspectives in order to: (1) clarify the questions at stake, and (2) find solutions, even if these remain partial and provisory. In this respect, a new perspectivism should hold the different philosophical approaches together, while respecting their differences and being open to the creation of new ones. This heterogeneity provides a wide set of perspectives, not only about current chemical practices but also about the ways to explore them.

Each approach is a *resource* for studying chemistry and for reflecting upon what *doing philosophy of science* can mean. We thus need to study: (1) the language of chemists, as well as the history of chemistry as a record of discoveries and conceptual and experimental innovations, (2) the balance between justifications for beliefs from logical reasoning and from local truth conditions and criteria, as well as social and political influences on beliefs, (3) chemical symbols, as well as chemical transformation of the world, (4) interrelations between sciences, as well as those between sciences and humanity in general, (5) chemistry in industry, as well as academic research, (6) networks of communication, as well as chemical instrumentation, (7) history of chemistry as well as history *tout court*, (8) philosophy of chemistry and of other sciences, as well as anthropology of science, and (9) the many other perspectives that will emerge for exploration and construal.

Chemistry is neither exhaustively social nor purely logical. Notwithstanding their ever-open dimensions, the definition and the study of chemistry need *cooperation* between heterogeneous perspectives that

explore their multifarious faces. “Socially embedded” does not amount to “socially determined”. Nor does “truth justification procedure” mean that “chemistry is a primarily theory-oriented activity only”. Each approach stresses a particular side of the study among many others. The challenge is to hold those perspectives together without necessarily referring to any kind of consilience or teleology and, above all, by avoiding any overly enthusiastic form of assimilation. Following this line, all the resources should be taken into account. There are textbooks, archives, chemical literature, case studies, laboratories, instruments, symbols, “paper tools” (iconographic representation, formula, pictures, diagrams, etc.), chemical concepts and devices, networks of communication, social laws and norms, human values, metaphysical assumptions, public opinion, factories and sites, human life and ethics, among many other factors. We have to envisage the circulation of concepts, methodologies, and devices from one domain to another, and to identify the questions at stake in relation to all this activity with the rest of human life.

Isabelle Stengers suggests distinguishing between two modes of propagation of concepts. The first is achieved through diffusion. In this case, the disciplinary origin of the concept is recognized, and we operate in the context of an openly metaphorical use. The second case evolves as an epidemic. The source of the concept is forgotten, and the concept is presented as “pure”, as cut off from natural language, and it appears as defined by the formalism of the science that it helps to organize (Stengers, 1987). In a complementary, though different perspective, Deleuze and Guattari give an account of a composite knowledge formation by putting forward the thesis of mobility inherent to the concept that joins together components that come from other concepts, which answers other problems and other supposed co-creations. According to them, a concept does not require only one problem under which it alters or replaces preceding concepts but, rather, a *crossroads of problems* in which it is combined with other coexistent concepts (Deleuze and Guattari, 1991, 1996).

This approach is all the more relevant because it entails that chemists have to face new problems and are formulating new questions and framing new devices, concepts, and methods in order to deal with these problems. For instance, they have to reshape their ways of doing chemistry in order to control the environmental impact of their activities. Additionally, ethical concerns percolate through chemical grounds, while chemistry provides philosophers with new problems that may drive an evolution of ethics itself (see Godard’s paper in this volume). A careful philosophical study is therefore needed to follow this interrelation between chemistry and ethics. Chemists also have to deal with mereological issues, such as

the integration of the size of nanoparticles into previous compositional and structural schemes in order to think about chemical reactivity. The way they think about a chemical “whole”, its parts, and the surroundings is, therefore, also changing (Llored, forthcoming). Additionally, the integration of chemistry into the work of the material sciences, biology, physics of the environment and space, and toxicology forces chemistry to adapt its mode of existence to such multifarious backgrounds.

Epistemologists and philosophers should scrutinize all these issues by employing different approaches. They can scrutinize how new quantum models arise and gain their theoretical legitimacy, while keeping in touch with the coupling of instruments that enable chemists to follow a transformation (as that of mass spectrometry and liquid chromatography, for example). As Stéphane Bouchonnet and Saïd Kinani point out in this volume, philosophers and historians should investigate the way chemists synthesize a “blank matrix” in order to give sense to the determination of a chemical quantity. In doing so, they should query how models, norms, metrology, and societal expectations hold together at a particular time. They can investigate how chemists and (eco)toxicologists work with one another in order to assess the toxicology of a mixture of compounds and how, in turn, both this knowledge and those analytical methods influence new concepts, such as the life cycle of a product or that of an ecodesign for a new community.

The “practice turn” in contemporary philosophy, the sociology of sciences, and the “symmetric anthropology” of science have already emphasized the above-mentioned dynamic aspects of sciences, while advocating a return to the study of instruments and laboratory life. Many prominent researchers, such as Michael Lynch, Karin Knorr Cetina, Bruno Latour, Andrew Pickering, Ian Hacking, Michel Callon, David Bloor, Steve Woolgar, to name only a few, have widened and deepened our views on the sciences. However, these crucial works were mainly concerned with physics and sometimes with biology, but rarely with chemistry. Is it so surprising? I do not think so. Chemistry had to fight its way against other sciences in order to be acknowledged as an independent discipline with its own concepts and methods. In the same vein, the philosophy of chemistry needs to find its place within mainstream philosophy of science. Things are changing thanks to the works proposed by the philosophers of chemistry themselves and because of the evolution of our models and understanding of sciences and society.

This is not the way the story ends. We do not simply have to connect researchers from heterogeneous fields and to integrate chemists into philosophical areas *as if* chemistry were not transforming our world. We

also have to understand that chemical instruments are not solely “allies” in discursive strategies. They also produce chemicals that change our lives, transform our society and values, and act upon the world. We *do not completely control* the consequences of this production and, thus, our future is already at stake. We sometimes succeed in determining the relative toxicity of chemicals. This is a matter of effort, skill, and creativity. But we are still investigating methods that could enable us to assess the toxicity of a mixture of compounds. Chemicals “A” and “B” can act upon us in such or such way, but the mixture “A + B” sometimes displays emergent effects. This is a familiar theme in pharmacology where the interaction between medicines is a matter of great importance. In their daily activities, chemists, nanochemists, and ecotoxicologists are essentially facing this kind of problem. In doing so, they allow for new sense to emerge from instruments, coupling of methods, and previous chemical and biological explanations and theories. We thus need to scrutinize how those methods are construed in order to better understand the role and the status of what Rom Harré calls the “apparatus/world complex”.

Chemistry is not about the world as it is, allegedly independently of us. In the same vein, chemistry is not about the projection of the knowing subject's categories, whatever may be the nature of this individual or collective knowing subject, and no matter how the categories may be considered, that is, ahistorically or as evolving with time. Rather, chemistry is about the interaction between subjects and the world. Rom Harré reminds us that we should not ignore the contribution of our apparatus to the form and qualities of the phenomenon. According to Harré, the question “In what form does metallic sodium exist before the electrolysis begins?” is illegitimate, in so far as metallic sodium is not something preexisting but is, rather, afforded by our actions! So, according to Harré, back inference from phenomena created in Bohrian artifacts, complexes of world and equipment, is problematic since there are ontological questions that remain to be solved (Harré, 2003). Chemistry and the other physical sciences are, therefore, about “affordances”. We know what “the apparatus/world complex” affords, no more and no less. Rom Harré invites us to recast the metaphysics that informs our experiments, and he paves the way for further investigations in this direction that could be based on chemistry. Following his line of reasoning, I claim that all we know concerns the products of interactions, no matter how real, dispositional, or functional their status may be in the economy of knowledge. It is only too easy to take plausible explanatory models of the unknown inwardness of natural beings for reality.

In a complementary perspective, Andrew Pickering and Ursula Klein are querying our dialectic of “resistances and accommodations” to use Pickering’s expression (Pickering, 1993). Klein never ceases to analyze the relations between materials and our conceptions about them (Klein and Spary, 2010). She even identifies forms of independence between what she calls “materiality” and theories, depending on the periods and the problems at stake. Following this line of reasoning, chemistry could provide philosophers with a new understanding of our interaction with the world and could enable them to develop new models of human knowledge and action. This is why we need to better understand the metrological aspects of chemistry, the construction of instruments, the coupling of methods, the ways conclusions are drawn from chemical analysis, and the role of “blank matrix”. This is why the first part of the volume emphasizes methodological and instrumental aspects, while the second part concerns methodologies and the last part concerns concepts. This is also the reason why Harré, Klein, Chamizo, Nordmann, Bouchonnet, Kinani, Renard, Berthet, Bitbol and I are querying the instrumental aspects of chemical practice within this volume. In line with Holmes and Levere (2000), our collective work is a plea for further investigation regarding the manner in which instruments and materials are co-adapted within chemical works, in order to understand the world that we are transforming. In this respect, Rom Harré proposes that we should reshape our understanding of instruments by construing a new metaphysics for experiments (Harré, 1986, 2003, 2004). The door is thus open to chemistry in the philosophical realm.

Undeniably, we are changing the world by means of chemicals. We are transforming ecosystems, society, the stratosphere, and the human body. We, therefore, have to face the consequences of our actions. This is why a pragmatic study of chemistry must be developed. Accordingly, in this volume, we have tried to integrate this way of thinking into a global reflection about chemistry. This is also the reason why we propose studies about sustainable chemistry and chemical risks. My aim, in suggesting this collection of studies, was to integrate these perspectives into the domain of the philosophy of chemistry by reflecting upon current chemical practices. Godard, Rico-Lattes, Maxim, and Caillol have thus opened the door for further studies, particularly regarding: (1) the anthropology of chemical risks, (2) the epistemology of sustainable chemistry, and (3) the interplay between ethics, moral philosophy, and science.

I repeat once again that we know the actions of the molecules “A” and “B” but not those of their mixture. We also know that their joint toxicity depends upon the size of the particles and not solely upon their composition.

Toxicity, that is to say the dangerous action upon life of our own productions, partly or fully escapes our expectations and their foundation in our rational schemes. The world cannot be considered to be quiet and inert. We act upon the world and we have to face the consequences of our actions. The world thus enters into the laboratory from the very outset of chemical design (Llored, 2011). This aspect of chemical work should be taken into account by epistemologists and philosophers, in order to grasp the significance of the changes evident in current chemistry.

This is precisely why we need to connect the different existing philosophical perspectives, while creating new ones. Symbols are as important as actions. Philosophy suffers from too many dichotomies. The challenge, therefore, is to create and to allow different points of view to co-exist without assimilating them into a unique scheme. If we accept, with Rom Harré (2006), that all boundaries between scientific realms or between philosophical approaches are “complementary”, in so far as they use different modes of access (cognitive or “instrumentariums”), and if we accept, with Quine (1966), that each realm has its own methods, concepts, representations, and “relative ontology”, then we can take our distance from those dichotomies. So what about the alleged dichotomy between “analytical philosophy” and “continental philosophy”? Division is a useful tool for organizing the content of education programmes and for beginning conceptual analysis, but not for much else. In the same vein, philosophers interested in practical studies sometimes reject the idea of philosophy as revealing the logical forms of propositions, and conversely. The trouble is that we need both approaches and many others, all directed to the same problems of interpretation and understanding of practices like chemistry. *Connections are translations: they transform the approaches engaged by them.* Connections enable the different perspectives that are at stake to co-evolve, sometimes by strengthening their arguments, sometimes by changing their conceptual basis. To the extent that the future of life is at state and that philosophy of science needs to incorporate moral considerations, we should question these dichotomies and look for new concepts, innovative methods, and novel practices, that is to say, for new ways of doing philosophy of science *tout court*.

Following Gilbert Hottois (1996, 2004, 2013), who first introduced the term “technosciences”, we can conclude that studying sciences philosophically needs: (1) no “logothetical” primacy, (2) no primacy for human interests and social constructions because of the way the world resists our incursions, and (3) multifarious temporalities within which we engage in it. We have to consider *homo loquax* as well as *homo faber*. Philosophers should not reduce practices to their symbolic aspects but

must also account for their operative and performative transformation of the world. Within some contexts, the interplay between technique and science is so strong that it practically becomes impossible to draw a sharp delineating line between them. We must, therefore, grasp the emergent whole philosophically. Hottois reminds us that technoscience is primarily concerned with the mutation and the possible disappearance of humankind due to the effects of our actions on the world. We have thus to recontextualize our human condition within the temporality of the universe, from the perspective of our possible extinction. According to Hottois, we must avoid the philosophical mistake of reducing the understanding of technosciences to anthropological and antropomorphic standpoints. He, therefore, pleads for a “trans-anthropological” account of technosciences. In this respect, we should consider the radical alterity and openness of the future in the long run. No one can actually foresee what our actions, including those that are chemically based, are likely to bring about in an extremely remote future. The power and the possibilities involved in technoscience go beyond the classical understanding of “technique” as the externalization of latent human capacities, as well as beyond the teleology and the eschatology related to it (Hottois, 1996). The technosciences go beyond our anthropological differences from other species, namely the symbolic singularity of our forms of life. This anthropological stance is itself shaken by internal and external non-symbolic processes. We have to accept that the naturalization of the anthropological difference is primarily concerned with its operationalization. Theoretical descriptions, symbolizations of all kinds, and the reflections they enable can only interact with this operationalization, without either anticipating it or being able to replace it (Hottois, 1996, 2004).

The naturalization of our anthropological difference from the rest of the universe is the result of a natural, physical, causal, and non-necessary operativity, that is to say, it is open to the intervention of technique. Symbols are not a starting point. The remote future is a challenge to conceptualization. We should not deprive ourselves from considering its development. However, the temporality engaged by technosciences can neither be symbolized nor historicized from the outset: we cannot put its actualization aside. The time of eschatology and imagined utopias has vanished. Our relation with the world is not basically symbolic but is, rather, technical and operative. We participate in the production of the future. We interfere with the processes of nature and society by resistances and accomodations. We must, therefore, recognize that the dynamic of anthropological processes is at least partly independent from symbolic activities (Hottois, 1996). We have thus to contrive a new interplay



between philosophy, techniques, and the sciences. The operative universality of technosciences is likely to interest philosophers in search for universality. However, universality has to be understood from the viewpoint of an operative causality. The technosciences should require the universality of philosophy as the unique appropriate kind of symbolic interrelation (Hottois, 1996, 2012). Technosciences explore the cosmos, nature, and living systems; they are non- or trans- anthropological and, sometimes, they are considered to be inhuman. A practical epistemology and philosophy of science is needed to articulate symbols and technosciences differently and to face the crucial societal choices and ethical problems of the present. The epistemological studies of practices should provide philosophers and other members of society with interesting information that will enable them to take distance from hasty idealizations and to sharpen the debate. In this respect, chemistry should help philosophers to create new bridges between symbols and action, representing and intervening (Llored, 2012). This is what this collective book partly aims to do.

This volume is about cooperation between researchers and it calls for further studies. These interconnected perspectives turn out to be valuable tools that allow philosophers to contrive new concepts or to reshape older ones, while rethinking the relationship between ways of doing science and philosophy. The cooperation between philosophical approaches is a good way to make a new understanding of science, technology, and society and of their interrelation, *co-emerge within a creative act*. It is also a chance for developing new arguments within each perspective and to contrive novel approaches. In doing so, one should take the constitutive role of the mode of access – cognitive or instrumental – into account in order to investigate the interplay between phenomena and knowledge at a particular time and to find solutions to the new challenges that chemists, as well as lay people, have to cope with in order to preserve (bio)diversity and to think about life *from within* our world (Bitbol, 2010). This is also why ethics, philosophy of science, political, and moral philosophies are likely to interact. But this aspect will be further studied in a forthcoming second collective volume.



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